



Full wwPDB EM Validation Report ⓘ

Jun 27, 2026 – 08:18 am BST

PDB ID : 9ROR / pdb_00009ror
EMDB ID : EMD-54129
Title : Assembly intermediate of human mitochondrial ribosome small subunit bound to METTL15 and RBFA (Outward conformation) (State M3)
Authors : Khawaja, A.; Singh, V.; Shiriaev, D.I.; Rorbach, J.
Deposited on : 2025-06-21
Resolution : 3.64 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

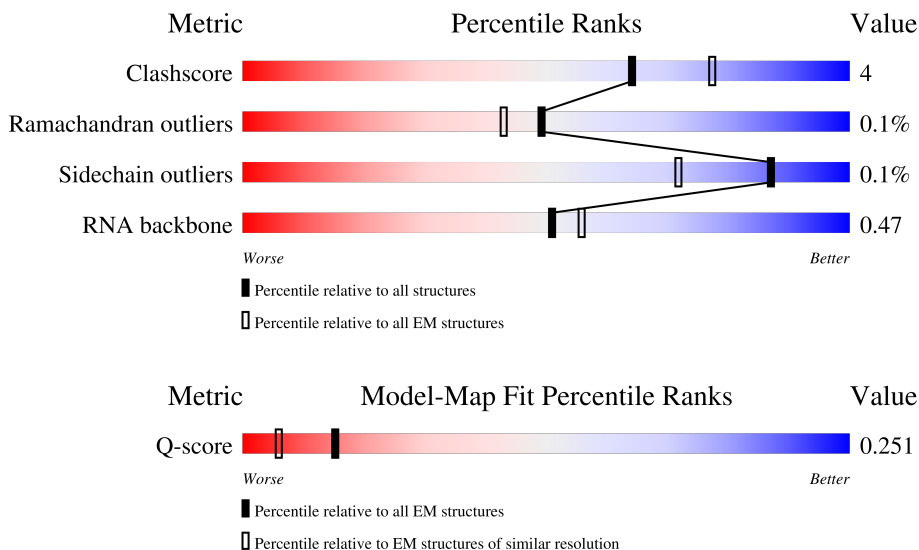
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




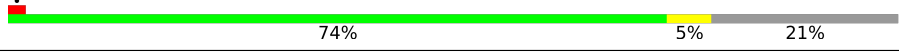

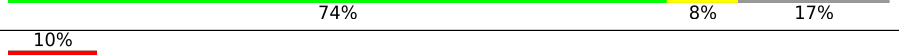
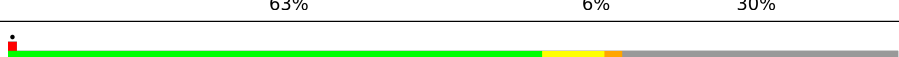
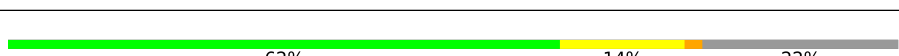







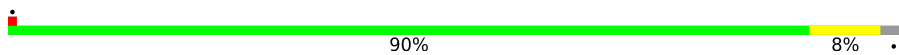

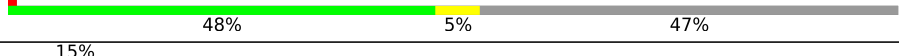


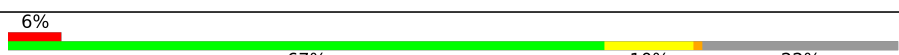
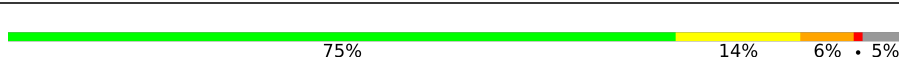

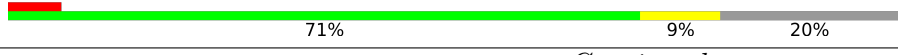



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11633 (3.14 - 4.14)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	218	
2	1	323	
3	3	199	

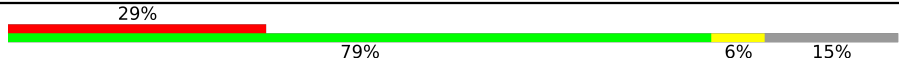

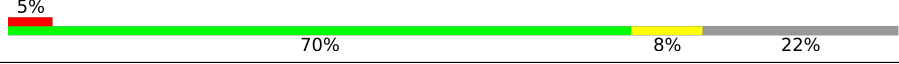
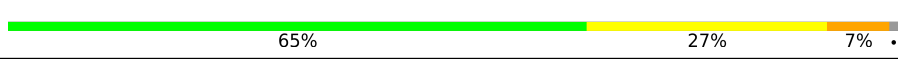
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Mol	Chain	Length	Quality of chain
4	B	296	
5	C	167	
6	E	125	
7	F	242	
8	H	201	
9	I	194	
10	J	138	
11	K	128	
12	L	257	
13	M	137	
14	N	130	
15	O	258	
16	P	142	
17	R	360	
18	S	190	
19	T	173	
20	U	205	
21	W	187	
22	X	398	
23	Y	395	
24	D	430	
25	G	396	
26	Q	87	
27	V	414	
28	Z	106	

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Mol	Chain	Length	Quality of chain
29	4	689	
30	a	343	
31	b	407	
32	A	954	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	FES	P	201	-	-	X	-

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 128254 atoms, of which 59425 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 28S ribosomal protein S34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	0	210	3509	1108	1757	333	306	5	0	0

- Molecule 2 is a protein called 28S ribosomal protein S35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	1	276	4507	1419	2269	381	427	11	0	0

- Molecule 3 is a protein called Aurora kinase A-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	3	70	1324	401	699	134	89	1	0	0

- Molecule 4 is a protein called 28S ribosomal protein S2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	B	225	3643	1164	1815	331	323	10	0	0

- Molecule 5 is a protein called 28S ribosomal protein S24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	C	132	2171	699	1088	195	185	4	0	0

- Molecule 6 is a protein called 28S ribosomal protein S6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	E	115	1839	574	929	165	167	4	0	0

- Molecule 7 is a protein called 28S ribosomal protein S7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	F	200	3344	1049	1699	297	288	11	0	0

- Molecule 8 is a protein called 28S ribosomal protein S10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	H	140	2335	745	1183	194	210	3	0	0

- Molecule 9 is a protein called 28S ribosomal protein S11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	I	134	2014	624	1023	185	178	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	184	5F0	ASN	variant	UNP P82912

- Molecule 10 is a protein called 28S ribosomal protein S12, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	J	108	1723	521	884	169	143	6	0	0

- Molecule 11 is a protein called 28S ribosomal protein S14, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	K	101	1747	537	885	179	141	5	0	0

- Molecule 12 is a protein called 28S ribosomal protein S15, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	L	174	2993	925	1540	270	251	7	0	0

- Molecule 13 is a protein called 28S ribosomal protein S16, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	M	119	1904	594	963	184	157	6	0	0

- Molecule 14 is a protein called 28S ribosomal protein S17, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	N	110	1796	562	928	156	147	3	0	0

- Molecule 15 is a protein called 28S ribosomal protein S18b, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
15	O	194	3164	1019	1565	295	278	7	0	0

- Molecule 16 is a protein called 28S ribosomal protein S18c, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	P	97	1587	501	806	134	138	8	0	0

- Molecule 17 is a protein called 28S ribosomal protein S22, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	R	295	4837	1533	2428	413	455	8	0	0

- Molecule 18 is a protein called 28S ribosomal protein S23, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	S	135	2226	716	1115	198	196	1	0	0

- Molecule 19 is a protein called 28S ribosomal protein S25, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	T	168	2764	877	1393	239	244	11	0	0

- Molecule 20 is a protein called 28S ribosomal protein S26, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	U	176	2987	916	1499	301	267	4	0	0

- Molecule 21 is a protein called 28S ribosomal protein S28, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	W	100	1591	498	802	141	146	4	0	0

- Molecule 22 is a protein called 28S ribosomal protein S29, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
22	X	352	5693	1822	2844	499	517	11	0	0

- Molecule 23 is a protein called 28S ribosomal protein S31, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
23	Y	121	1993	662	970	168	191	2	0	0

- Molecule 24 is a protein called 28S ribosomal protein S5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
24	D	322	5189	1617	2614	483	462	13	0	0

- Molecule 25 is a protein called 28S ribosomal protein S9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
25	G	310	5110	1627	2547	456	466	14	0	0

- Molecule 26 is a protein called MRPS21 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
26	Q	83	1441	439	731	144	120	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	1	ACE	-	acetylation	UNP A0A2J8VEN6

- Molecule 27 is a protein called 28S ribosomal protein S27, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
27	V	352	5770	1853	2886	480	539	12	0	0

- Molecule 28 is a protein called 28S ribosomal protein S33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
28	Z	85	1459	462	737	128	128	4	0	0

- Molecule 29 is a protein called Pentatricopeptide repeat domain-containing protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
29	4	588	9534	3053	4766	808	879	28	0	0

- Molecule 30 is a protein called Putative ribosome-binding factor A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
30	a	155	2445	766	1225	212	235	7	0	0

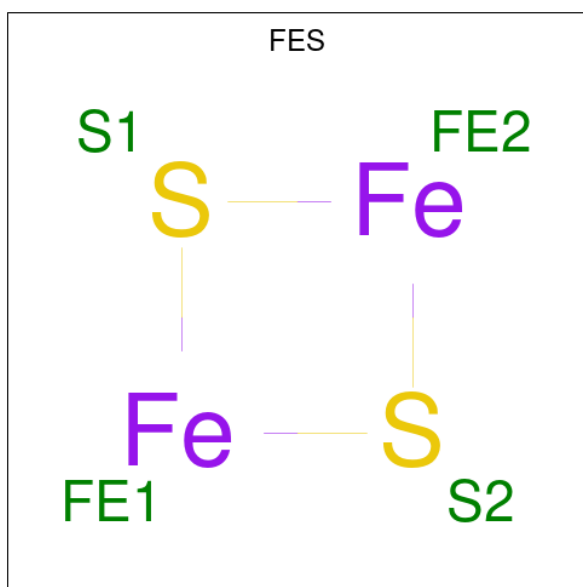
- Molecule 31 is a protein called 12S rRNA N4-methylcytidine (m4C) methyltransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
31	b	319	5062	1580	2564	449	455	14	0	0

- Molecule 32 is a RNA chain called 12S mitochondrial rRNA.

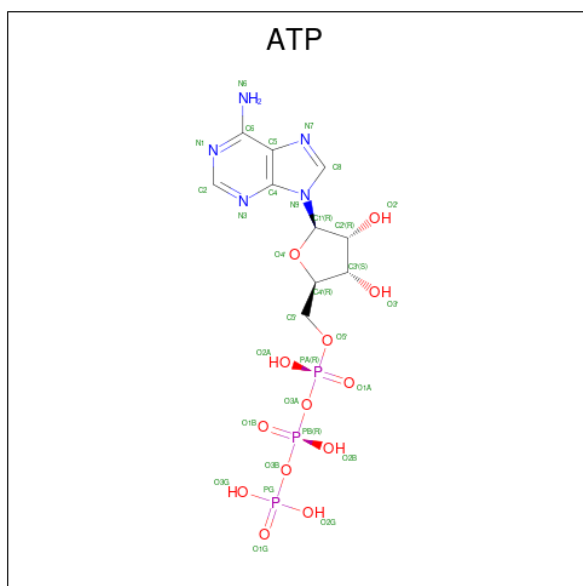
Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
32	A	948	30360	9032	10223	3627	6530	948	0	0

- Molecule 33 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



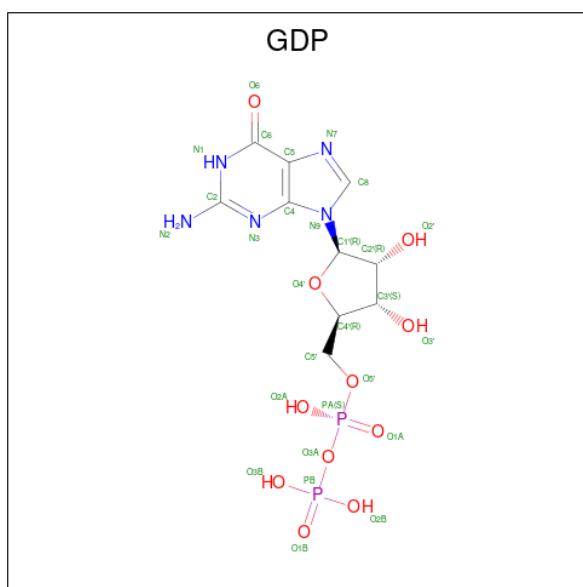
Mol	Chain	Residues	Atoms			AltConf
33	P	1	Total	Fe	S	0
			4	2	2	
33	T	1	Total	Fe	S	0
			4	2	2	

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



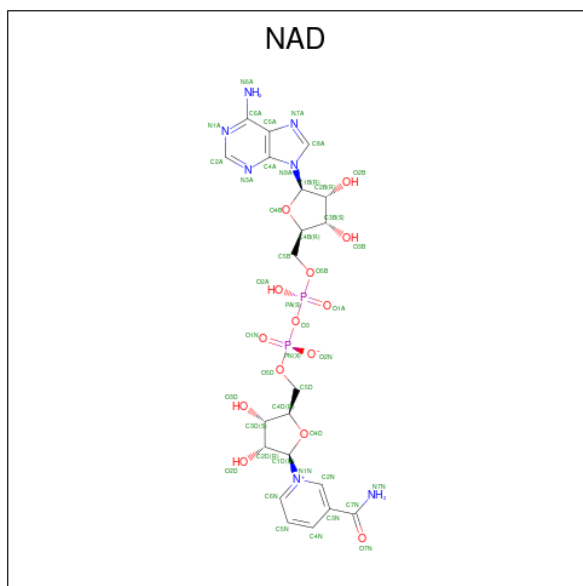
Mol	Chain	Residues	Atoms					AltConf	
34	X	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 35 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



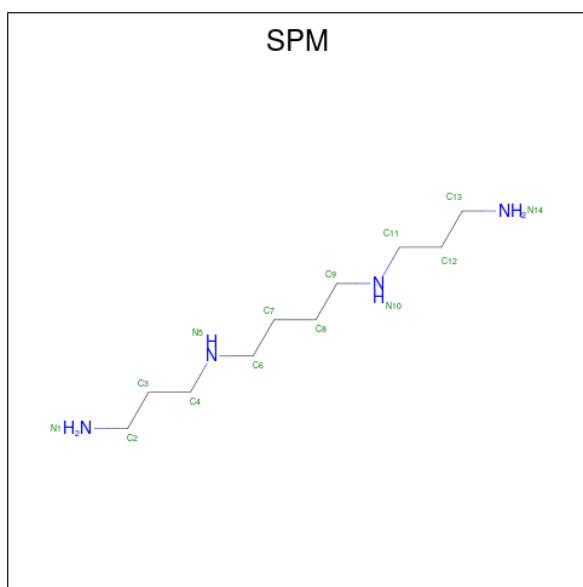
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
35	X	1	38	10	10	5	11	2	0

- Molecule 36 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
36	A	1	70	21	26	7	14	2	0

- Molecule 37 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms		AltConf
37	A	1	Total	C N	0
			14	10 4	

- Molecule 38 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

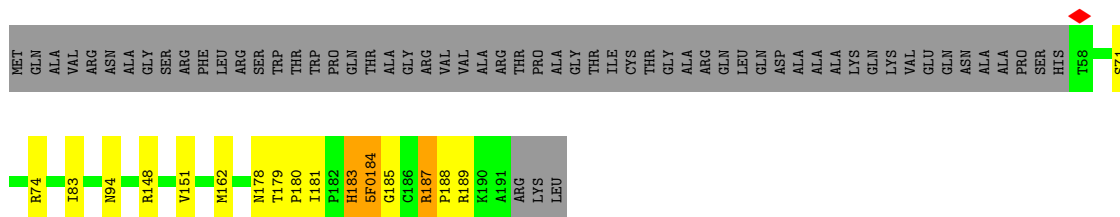
Mol	Chain	Residues	Atoms		AltConf
38	A	11	Total	Mg	0
			11	11	

- Molecule 39 is POTASSIUM ION (CCD ID: K) (formula: K).

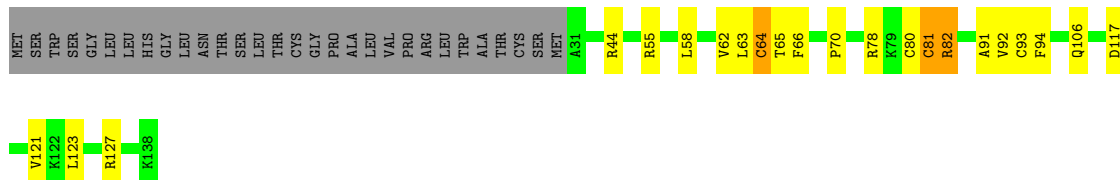
Mol	Chain	Residues	Atoms		AltConf
39	A	8	Total	K	0
			8	8	

- Molecule 40 is water.

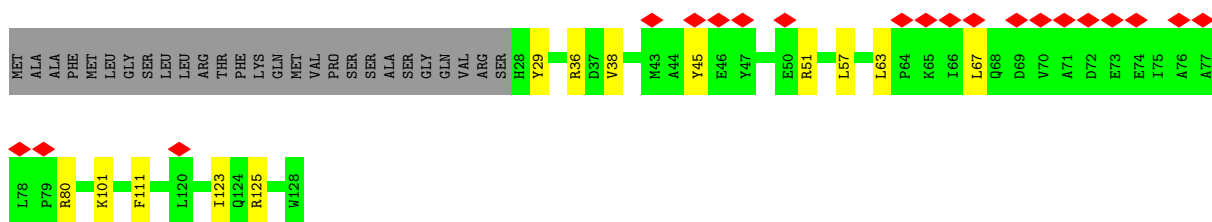
Mol	Chain	Residues	Atoms		AltConf
40	T	1	Total	O	0
			1	1	



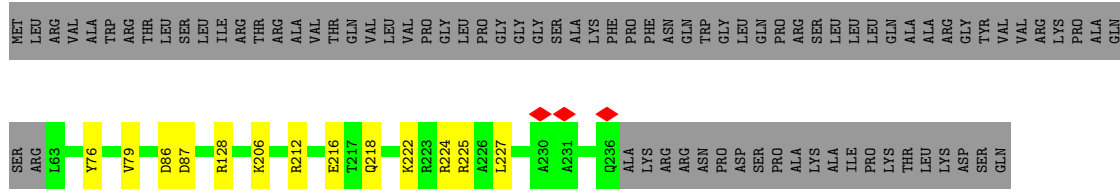
• Molecule 10: 28S ribosomal protein S12, mitochondrial



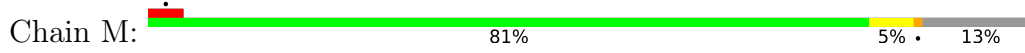
• Molecule 11: 28S ribosomal protein S14, mitochondrial



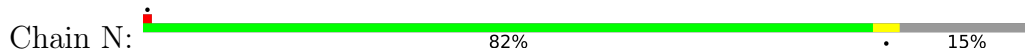
• Molecule 12: 28S ribosomal protein S15, mitochondrial

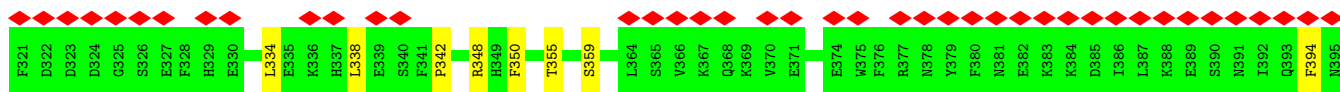


• Molecule 13: 28S ribosomal protein S16, mitochondrial

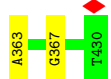
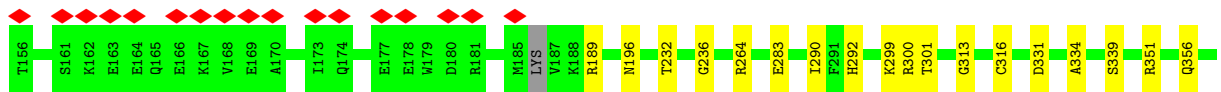
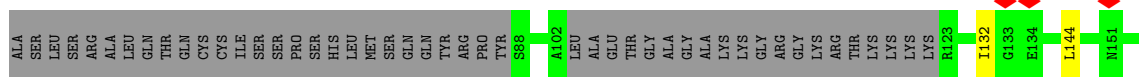
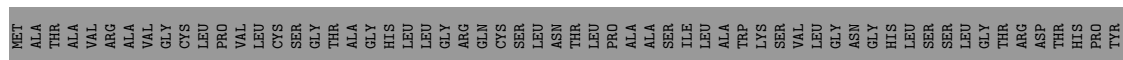


• Molecule 14: 28S ribosomal protein S17, mitochondrial

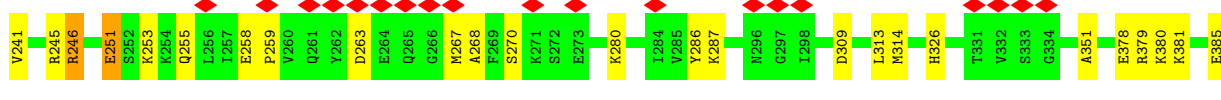
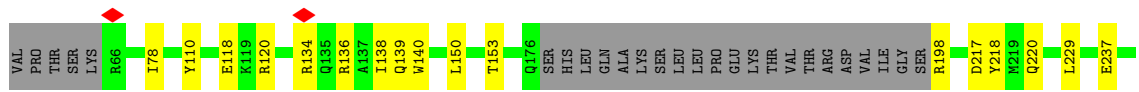
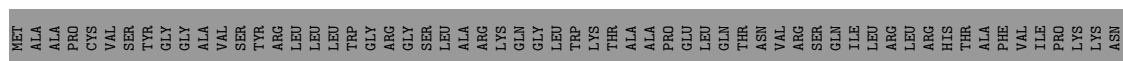




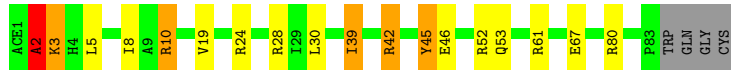
• Molecule 24: 28S ribosomal protein S5, mitochondrial



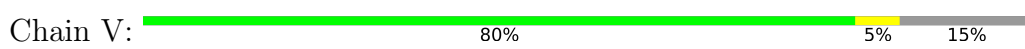
• Molecule 25: 28S ribosomal protein S9, mitochondrial

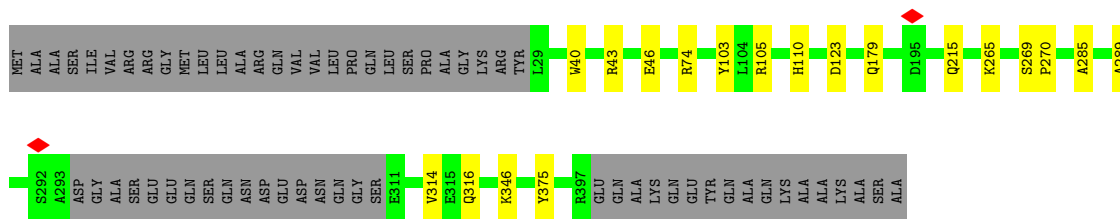


• Molecule 26: MRPS21 isoform 1



• Molecule 27: 28S ribosomal protein S27, mitochondrial

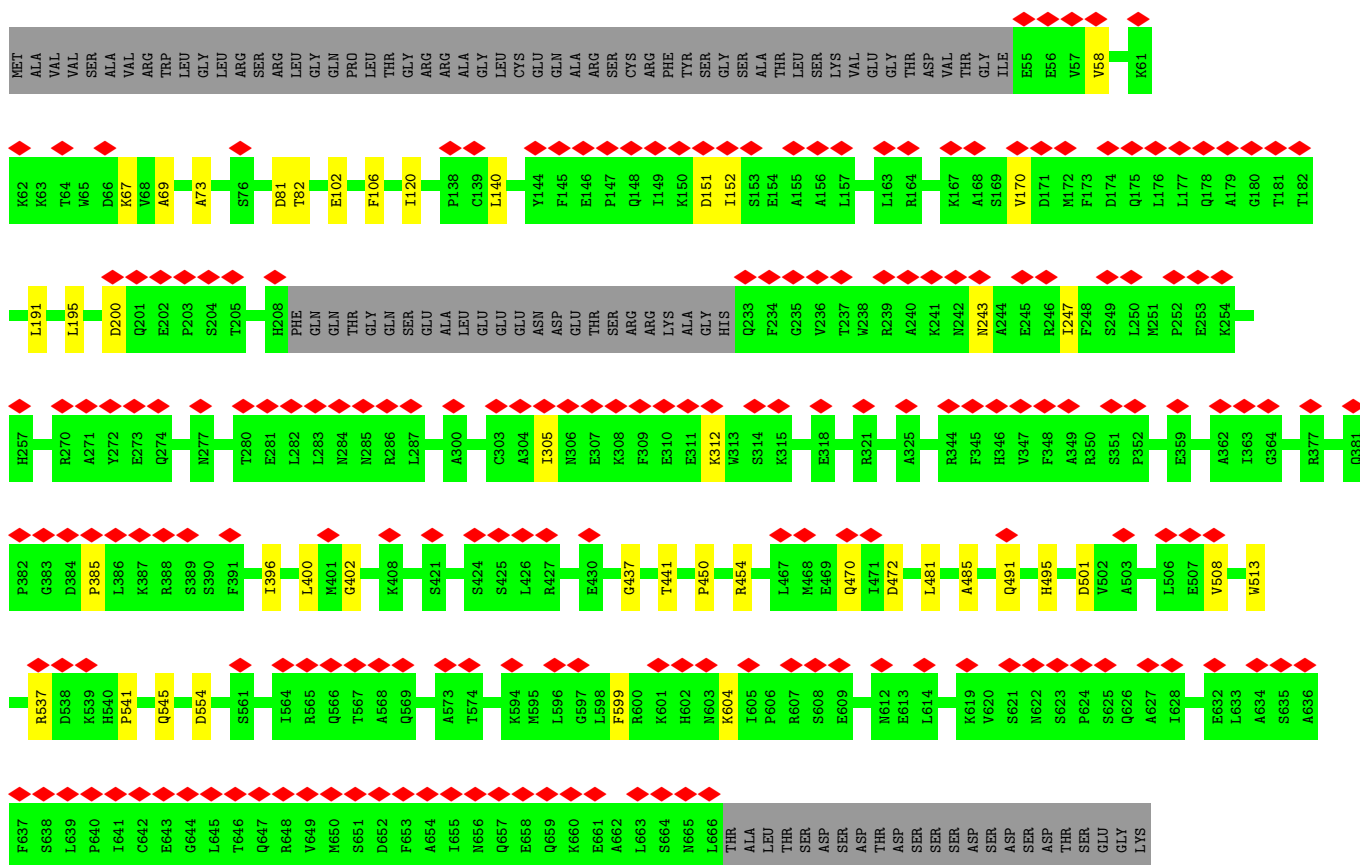
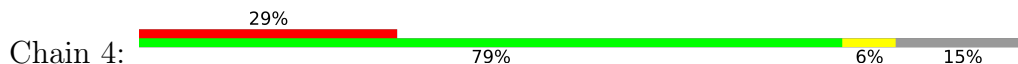




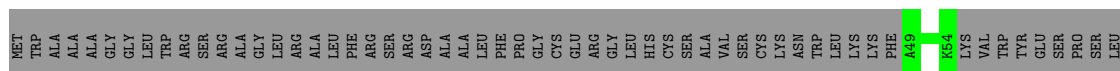
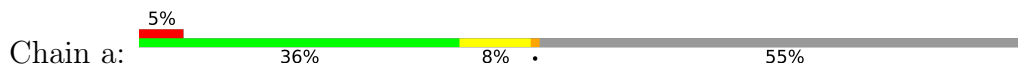
• Molecule 28: 28S ribosomal protein S33, mitochondrial



• Molecule 29: Pentatricopeptide repeat domain-containing protein 3, mitochondrial



• Molecule 30: Putative ribosome-binding factor A, mitochondrial



A1266	A1357	A1458	A1546
U1269	A1358	A1461	U1547
A1272	U1359	G1462	A1548
G1273	A1365	G1463	G1549
A1276	C1366	G1464	A1557
A1277	U1369	C1465	G1562
C1278	U1373	C1466	U1563
C1279	A1374	U1467	A1564
A1283	C1375	A1470	A1565
U1284	C	G1474	U1568
G1285	C	A1478	G1569
C1290	A	C1479	U1570
U1291	G1380	A1480	U1571
A1292	A1381	C1481	A1572
C1293	A1382	A1482	A1573
A1296	A1383	C1483	G1574
G1297	A1384	G1484	G1582
U1298	C1385	A1485	A1583
A1299	U1386	C1486	A1584
A1300	A1387	A1482	G1591
G1307	G1388	A1492	G1594
U1308	G1389	C1493	G1595
A1309	U1400	C1494	A1596
G1315	G1401	C1495	C1597
U1316	A1402	G1503	G1598
A1317	C1405	U1504	A1599
A1318	A1412	A1505	A1600
A1319	U1413	U1506	C
U1325	C1414	A1512	
A1326	A1417	C1518	
G1327	G1418	A1519	
G1328	G1419	U1520	
U1329	U1420	U1521	
C1330	G1421	U1522	
A1331	G1422	A1523	
U1335	U1426	A1524	
G1336	A1430	C1525	
U1337	A1430	U1526	
A1338	G1442	A1527	
C1341	U1443	A1530	
C1342	A1444	C1531	
A1343	G1445	C1532	
G1350	A1446	C1533	
G1351	G1447	A1536	
C1352	U1448	C1537	
A1353	U1452	G1538	
A1354	U1456	C1539	
G1457	U1456	A1540	
		U1541	
		G1457	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10529	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.038	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	495.0, 495.0, 495.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.825, 0.825, 0.825	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, FES, 5F0, K, SPM, ACE, GDP, MA6, NAD, 5MC, ATP, 5MU, B8T

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.07	0/1798	0.20	0/2436
2	1	0.19	0/2285	0.30	0/3090
3	3	0.06	0/636	0.20	0/839
4	B	0.06	0/1871	0.19	0/2531
5	C	0.06	0/1113	0.19	0/1505
6	E	0.06	0/926	0.19	0/1252
7	F	0.31	0/1681	0.40	1/2255 (0.0%)
8	H	0.27	0/1178	0.40	0/1598
9	I	0.26	0/1001	0.56	3/1350 (0.2%)
10	J	0.88	0/855	0.96	2/1148 (0.2%)
11	K	0.07	0/880	0.23	0/1182
12	L	0.25	0/1477	0.36	0/1974
13	M	0.22	0/962	0.38	1/1293 (0.1%)
14	N	0.07	0/886	0.21	0/1199
15	O	0.07	0/1655	0.22	0/2254
16	P	0.06	0/798	0.19	0/1070
17	R	0.06	0/2456	0.19	0/3317
18	S	0.06	0/1138	0.16	0/1533
19	T	0.16	0/1402	0.29	0/1883
20	U	0.06	0/1510	0.18	0/2025
21	W	0.06	0/801	0.18	0/1079
22	X	0.07	0/2921	0.22	0/3954
23	Y	0.59	0/1054	0.69	0/1421
24	D	0.07	0/2625	0.19	0/3518
25	G	0.30	0/2618	0.39	0/3507
26	Q	0.64	0/718	1.01	3/955 (0.3%)
27	V	0.06	0/2944	0.18	0/3978
28	Z	0.09	0/737	0.23	0/980
29	4	0.07	0/4877	0.22	0/6598
30	a	0.39	0/1236	0.69	3/1666 (0.2%)
31	b	0.07	0/2542	0.20	0/3427
32	A	0.16	0/22398	0.28	2/34866 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.21	0/71979	0.32	15/101683 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	F	0	2
9	I	0	5
10	J	0	3
12	L	0	1
13	M	0	1
23	Y	0	1
26	Q	0	6
30	a	0	2
All	All	0	21

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	180	PRO	O-C-N	-13.37	107.05	123.10
10	J	64	CYS	N-CA-C	8.48	120.98	108.60
10	J	64	CYS	N-CA-CB	-7.78	99.48	111.46
30	a	98	GLY	N-CA-C	-7.72	103.41	112.83
32	A	1387	A	C2'-C3'-O3'	6.89	119.84	109.50
32	A	1386	U	O3'-P-O5'	6.75	114.13	104.00
26	Q	2	ALA	O-C-N	6.49	133.38	123.00
7	F	163	LYS	N-CA-CB	6.40	119.29	110.01
30	a	92	ARG	N-CA-C	-6.25	105.59	112.72
9	I	180	PRO	CA-C-N	5.84	132.94	122.13
9	I	180	PRO	C-N-CA	5.84	132.94	122.13
26	Q	45	TYR	N-CA-CB	5.67	118.71	109.69
26	Q	39	ILE	N-CA-C	-5.57	104.94	110.62
30	a	122	VAL	N-CA-CB	5.49	116.52	110.53
13	M	26	CYS	CB-CA-C	-5.05	101.49	111.60

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	F	166	ARG	Sidechain
7	F	234	ARG	Sidechain
9	I	183	HIS	Mainchain
9	I	184	5F0	Peptide,Mainchain
9	I	187	ARG	Sidechain
9	I	189	ARG	Sidechain
10	J	127	ARG	Sidechain
10	J	44	ARG	Sidechain
10	J	82	ARG	Sidechain
12	L	225	ARG	Sidechain
13	M	29	ARG	Sidechain
26	Q	10	ARG	Sidechain
26	Q	2	ALA	Peptide
26	Q	24	ARG	Sidechain
26	Q	28	ARG	Sidechain
26	Q	42	ARG	Sidechain
26	Q	80	ARG	Sidechain
23	Y	348	ARG	Sidechain
30	a	92	ARG	Sidechain
30	a	94	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1752	1757	1757	9	0
2	1	2238	2269	2269	16	0
3	3	625	699	699	3	0
4	B	1828	1815	1815	8	0
5	C	1083	1088	1088	7	0
6	E	910	929	929	10	0
7	F	1645	1699	1699	18	0
8	H	1152	1183	1183	13	0
9	I	991	1023	1016	39	0
10	J	839	884	886	27	0
11	K	862	885	885	11	0
12	L	1453	1540	1540	8	0
13	M	941	963	963	7	0
14	N	868	928	928	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	1599	1565	1569	19	0
16	P	781	806	807	12	0
17	R	2409	2428	2428	9	0
18	S	1111	1115	1115	4	0
19	T	1371	1393	1395	10	0
20	U	1488	1499	1499	5	0
21	W	789	802	802	6	0
22	X	2849	2844	2844	24	0
23	Y	1023	970	970	11	0
24	D	2575	2614	2614	15	0
25	G	2563	2547	2545	34	0
26	Q	710	731	732	32	0
27	V	2884	2886	2885	11	0
28	Z	722	737	736	9	0
29	4	4768	4766	4766	27	0
30	a	1220	1225	1224	30	0
31	b	2498	2564	2564	20	0
32	A	20137	10223	10226	136	0
33	P	4	0	0	4	0
33	T	4	0	0	1	0
34	X	31	12	12	1	0
35	X	28	10	12	5	0
36	A	44	26	26	0	0
37	A	14	0	26	3	0
38	A	11	0	0	0	0
39	A	8	0	0	0	0
40	T	1	0	0	1	0
All	All	68829	59425	59454	482	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (482) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:105:CYS:CB	16:P:68:CYS:SG	2.27	1.23
10:J:64:CYS:HB3	10:J:81:CYS:SG	1.82	1.19
16:P:68:CYS:SG	33:P:201:FES:S2	2.39	1.19
9:I:179:THR:HG21	26:Q:39:ILE:HD13	1.24	1.17
26:Q:3:LYS:HE2	32:A:975:A:OP2	1.48	1.12
30:a:122:VAL:HG21	30:a:152:MET:HE2	1.25	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:91:ARG:CG	15:O:143:CYS:SG	2.41	1.08
6:E:105:CYS:HB3	16:P:68:CYS:SG	1.93	1.08
7:F:162:LEU:HD23	7:F:167:PHE:CZ	1.90	1.07
26:Q:3:LYS:HE2	32:A:975:A:P	1.97	1.04
9:I:183:HIS:HB3	32:A:1015:A:C8	1.98	0.99
15:O:91:ARG:HG3	15:O:143:CYS:SG	2.07	0.95
6:E:105:CYS:HB2	16:P:68:CYS:SG	2.05	0.94
30:a:122:VAL:HG21	30:a:152:MET:CE	2.00	0.92
26:Q:3:LYS:CE	32:A:975:A:OP2	2.19	0.91
19:T:141:CYS:SG	19:T:149:CYS:HB3	2.14	0.87
19:T:149:CYS:SG	33:T:201:FES:S1	2.71	0.87
30:a:122:VAL:CG2	30:a:152:MET:HE2	2.03	0.86
10:J:64:CYS:O	10:J:65:THR:HG23	1.76	0.85
10:J:80:CYS:SG	10:J:94:PHE:HA	2.17	0.84
9:I:183:HIS:HA	32:A:1015:A:O4'	1.80	0.82
9:I:179:THR:CG2	26:Q:39:ILE:HD13	2.08	0.80
15:O:91:ARG:HG2	15:O:143:CYS:SG	2.20	0.80
7:F:158:LEU:HD21	7:F:230:ALA:HA	1.63	0.79
30:a:122:VAL:CG2	30:a:152:MET:CE	2.60	0.78
9:I:179:THR:HG21	26:Q:39:ILE:CD1	2.09	0.78
26:Q:3:LYS:CE	32:A:975:A:P	2.74	0.76
32:A:806:C:OP2	32:A:807:A:N6	2.19	0.75
10:J:65:THR:N	10:J:81:CYS:SG	2.60	0.74
7:F:162:LEU:HD23	7:F:167:PHE:CE2	2.21	0.74
6:E:105:CYS:SG	16:P:68:CYS:SG	2.85	0.74
11:K:36:ARG:NH1	32:A:1235:U:OP1	2.20	0.74
15:O:91:ARG:HD2	15:O:143:CYS:SG	2.27	0.73
32:A:1175:G:O2'	32:A:1481:C:O2	2.06	0.73
9:I:183:HIS:CD2	32:A:1015:A:C4	2.77	0.72
15:O:91:ARG:CD	15:O:143:CYS:SG	2.78	0.72
27:V:40:TRP:O	27:V:43:ARG:NH1	2.23	0.71
29:4:170:VAL:HG21	29:4:195:LEU:HD21	1.72	0.71
10:J:64:CYS:HB3	10:J:81:CYS:CB	2.21	0.70
10:J:63:LEU:C	10:J:64:CYS:SG	2.74	0.70
19:T:132:ARG:NH1	19:T:136:LEU:O	2.24	0.70
32:A:688:A:O2'	32:A:689:U:OP2	2.07	0.69
2:1:235:ASN:ND2	2:1:237:GLU:OE2	2.26	0.69
9:I:188:PRO:HG2	26:Q:45:TYR:HA	1.75	0.69
13:M:43:ARG:NH1	32:A:853:C:O2'	2.27	0.67
12:L:76:TYR:O	12:L:79:VAL:HG22	1.93	0.67
25:G:150:LEU:O	25:G:153:THR:OG1	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:81:CYS:N	10:J:93:CYS:SG	2.68	0.67
18:S:7:GLU:N	18:S:7:GLU:OE1	2.28	0.67
10:J:92:VAL:HG11	10:J:121:VAL:HG22	1.77	0.66
1:O:78:ARG:NH2	1:O:142:VAL:O	2.29	0.65
9:I:185:GLY:CA	32:A:1013:A:H1'	2.26	0.65
7:F:233:ASN:O	7:F:234:ARG:C	2.39	0.65
9:I:185:GLY:O	32:A:1013:A:H1'	1.96	0.65
10:J:66:PHE:CD2	10:J:81:CYS:HA	2.31	0.65
32:A:1309:A:N6	32:A:1315:G:O6	2.30	0.65
15:O:73:VAL:O	15:O:109:ARG:NH2	2.30	0.65
26:Q:5:LEU:HB2	26:Q:8:ILE:HD11	1.77	0.65
9:I:187:ARG:NH1	26:Q:45:TYR:CE2	2.66	0.64
11:K:45:TYR:O	28:Z:44:LYS:NZ	2.30	0.64
9:I:183:HIS:CB	32:A:1015:A:C8	2.79	0.64
16:P:68:CYS:SG	33:P:201:FES:FE1	1.90	0.64
24:D:264:ARG:NH1	30:a:299:GLU:OE1	2.31	0.64
30:a:298:GLY:O	30:a:301:VAL:HG22	1.98	0.64
9:I:187:ARG:HG2	26:Q:45:TYR:HB2	1.79	0.63
22:X:333:GLY:O	22:X:337:LEU:HD23	1.99	0.63
28:Z:32:LYS:NZ	32:A:1400:U:OP1	2.31	0.63
9:I:183:HIS:CG	32:A:1015:A:C4	2.86	0.63
25:G:120:ARG:NH2	32:A:1307:G:O2'	2.32	0.63
32:A:1279:C:O2'	32:A:1296:A:N1	2.29	0.63
31:b:321:PHE:N	31:b:325:GLU:OE2	2.30	0.63
32:A:1505:A:N1	32:A:1546:A:N6	2.46	0.63
26:Q:3:LYS:HE2	32:A:975:A:O5'	1.98	0.62
32:A:1583:MA6:H93	32:A:1584:MA6:C2	2.29	0.62
17:R:208:ILE:O	17:R:214:ASN:ND2	2.32	0.62
7:F:158:LEU:HD23	7:F:171:PRO:HA	1.82	0.62
29:4:195:LEU:HD22	29:4:200:ASP:OD1	2.00	0.62
24:D:351:ARG:NH2	32:A:1118:A:O2'	2.31	0.62
30:a:97:ASN:HD21	30:a:129:LEU:HB2	1.65	0.61
15:O:94:CYS:SG	15:O:143:CYS:HB2	2.40	0.61
9:I:71:SER:O	9:I:74:ARG:NH1	2.34	0.61
29:4:470:GLN:NE2	29:4:472:ASP:OD2	2.34	0.61
23:Y:296:ASN:OD1	23:Y:298:PHE:N	2.34	0.61
28:Z:92:GLU:N	28:Z:92:GLU:OE1	2.34	0.61
16:P:68:CYS:CB	33:P:201:FES:S2	2.89	0.60
1:O:43:ARG:O	1:O:47:GLY:N	2.34	0.60
31:b:195:ARG:NH2	31:b:198:GLY:O	2.34	0.60
2:1:56:ARG:NH1	29:4:81:ASP:OD2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:183:HIS:CA	32:A:1015:A:O4'	2.49	0.60
32:A:1053:A:N1	32:A:1100:C:O2'	2.31	0.60
13:M:26:CYS:SG	19:T:149:CYS:HB2	2.40	0.60
32:A:1583:MA6:H93	32:A:1584:MA6:N1	2.16	0.60
32:A:700:A:N1	32:A:709:G:O2'	2.25	0.60
5:C:38:ARG:N	32:A:1265:C:OP2	2.33	0.60
31:b:162:THR:HG22	31:b:162:THR:O	2.01	0.59
26:Q:45:TYR:CE2	26:Q:46:GLU:O	2.55	0.59
28:Z:31:MET:O	28:Z:34:VAL:HG22	2.02	0.59
31:b:229:GLU:OE2	31:b:231:HIS:N	2.36	0.59
2:1:166:PRO:O	2:1:169:ARG:NH1	2.35	0.59
28:Z:91:LYS:NZ	32:A:1338:A:OP1	2.35	0.59
19:T:89:ASP:OD2	20:U:120:ARG:NH2	2.36	0.59
26:Q:2:ALA:O	26:Q:3:LYS:HG3	2.03	0.59
4:B:243:PRO:O	4:B:247:HIS:ND1	2.35	0.58
13:M:53:SER:H	13:M:67:ALA:HB3	1.69	0.58
10:J:80:CYS:HB3	10:J:93:CYS:SG	2.44	0.58
13:M:67:ALA:HB1	17:R:161:ILE:HG13	1.86	0.58
25:G:379:ARG:NH1	32:A:1452:U:OP1	2.37	0.58
29:4:151:ASP:OD1	29:4:152:ILE:N	2.36	0.58
7:F:104:LYS:NZ	32:A:1458:A:OP1	2.37	0.58
21:W:126:ARG:NH1	21:W:131:GLY:O	2.36	0.58
8:H:143:LEU:O	8:H:143:LEU:HD12	2.04	0.57
30:a:117:LEU:HD23	30:a:120:LEU:HD12	1.86	0.57
27:V:46:GLU:OE2	27:V:74:ARG:NE	2.37	0.57
31:b:266:ALA:O	31:b:269:THR:OG1	2.15	0.57
32:A:1214:A:N7	32:A:1353:A:N6	2.52	0.57
29:4:437:GLY:O	29:4:441:THR:HG23	2.04	0.57
32:A:1400:U:O2'	32:A:1401:G:OP1	2.23	0.57
16:P:68:CYS:HB2	33:P:201:FES:S2	2.44	0.57
30:a:122:VAL:HG11	30:a:140:TRP:CE3	2.40	0.57
4:B:180:ARG:NH1	4:B:185:PRO:O	2.38	0.57
27:V:103:TYR:O	27:V:105:ARG:NH2	2.38	0.57
27:V:105:ARG:NH1	32:A:1525:C:OP1	2.38	0.57
7:F:158:LEU:HD21	7:F:230:ALA:CA	2.33	0.56
14:N:38:TYR:OH	32:A:932:C:OP2	2.22	0.56
3:3:148:LYS:O	3:3:151:ARG:NH1	2.38	0.56
7:F:50:TYR:O	7:F:66:ARG:NH2	2.38	0.56
10:J:55:ARG:HD3	10:J:58:LEU:HD21	1.87	0.56
15:O:94:CYS:SG	15:O:143:CYS:CB	2.93	0.56
22:X:173:TYR:CD2	35:X:502:GDP:H2'	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:G:270:SER:OG	25:G:351:ALA:O	2.23	0.56
27:V:179:GLN:OE1	27:V:215:GLN:NE2	2.38	0.56
32:A:1106:C:O2'	32:A:1108:C:OP2	2.17	0.56
32:A:1230:C:OP2	32:A:1442:G:O2'	2.19	0.56
4:B:54:ASP:OD1	4:B:271:TYR:OH	2.24	0.56
9:I:179:THR:CG2	26:Q:39:ILE:CD1	2.77	0.56
16:P:65:CYS:SG	16:P:68:CYS:HB2	2.45	0.56
32:A:1226:C:O2'	32:A:1227:G:N7	2.37	0.56
25:G:385:GLU:OE1	25:G:389:ARG:NH1	2.38	0.56
32:A:1247:G:H21	32:A:1343:A:H61	1.52	0.56
6:E:15:ARG:NH2	20:U:182:ASP:OD1	2.39	0.55
22:X:383:LEU:HD13	25:G:314:MET:HE1	1.87	0.55
24:D:132:ILE:HG22	24:D:144:LEU:HD21	1.87	0.55
32:A:1106:C:O2'	32:A:1125:A:N6	2.39	0.55
25:G:134:ARG:O	25:G:136:ARG:NH1	2.38	0.55
32:A:934:G:O2'	32:A:940:A:N1	2.31	0.55
2:1:86:ARG:NH1	2:1:96:PRO:O	2.39	0.55
32:A:936:G:O6	32:A:1122:A:N6	2.38	0.55
32:A:1110:A:O2'	37:A:1702:SPM:H121	2.05	0.55
32:A:1247:G:N2	32:A:1343:A:H61	2.05	0.55
22:X:316:LEU:HD23	32:A:1373:U:O2'	2.07	0.55
24:D:301:THR:HG23	24:D:301:THR:O	2.06	0.55
25:G:217:ASP:OD1	25:G:218:TYR:N	2.40	0.55
26:Q:52:ARG:NH2	32:A:1591:C:OP1	2.38	0.55
10:J:66:PHE:CD2	10:J:81:CYS:SG	3.00	0.55
16:P:49:ASP:OD2	21:W:82:SER:OG	2.24	0.54
19:T:42:GLU:OE1	19:T:45:ARG:NH2	2.40	0.54
25:G:263:ASP:OD1	25:G:267:MET:N	2.40	0.54
22:X:241:GLY:HA3	35:X:502:GDP:H4'	1.89	0.54
10:J:66:PHE:CE2	10:J:81:CYS:HA	2.43	0.54
17:R:254:ASP:OD1	17:R:259:TYR:OH	2.25	0.54
32:A:1266:A:N1	32:A:1326:A:N6	2.55	0.54
32:A:1179:G:H4'	32:A:1180:U:OP2	2.07	0.54
31:b:326:ASP:OD2	32:A:1078:A:O2'	2.16	0.54
32:A:889:G:H21	32:A:902:G:P	2.31	0.54
32:A:905:A:O2'	32:A:907:A:OP1	2.26	0.54
10:J:80:CYS:SG	10:J:93:CYS:O	2.66	0.53
16:P:73:ASP:OD1	16:P:74:TYR:N	2.40	0.53
25:G:378:GLU:OE2	25:G:381:LYS:NZ	2.41	0.53
9:I:83:ILE:O	9:I:148:ARG:NH2	2.41	0.53
22:X:136:LEU:HD13	34:X:501:ATP:H4'	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:126:ALA:O	31:b:130:HIS:N	2.38	0.53
32:A:835:C:N4	32:A:851:A:OP2	2.32	0.53
10:J:64:CYS:HB3	10:J:81:CYS:HB3	1.90	0.53
9:I:185:GLY:O	32:A:1013:A:C1'	2.56	0.53
24:D:283:GLU:O	24:D:356:GLN:NE2	2.41	0.53
2:1:275:ASN:OD1	2:1:276:MET:N	2.42	0.53
7:F:158:LEU:HB3	7:F:169:GLN:HB3	1.91	0.53
20:U:80:ARG:O	20:U:84:GLU:N	2.42	0.53
31:b:164:ASP:O	31:b:315:ARG:N	2.42	0.53
3:3:150:THR:HG22	3:3:150:THR:O	2.09	0.52
22:X:382:PHE:CD1	25:G:314:MET:HE2	2.44	0.52
1:0:129:ARG:NH1	1:0:205:ALA:O	2.41	0.52
31:b:164:ASP:OD1	31:b:311:ARG:NH1	2.42	0.52
30:a:122:VAL:HG23	30:a:152:MET:CE	2.38	0.52
32:A:1211:G:H21	32:A:1354:A:H62	1.58	0.52
9:I:188:PRO:HB2	26:Q:45:TYR:N	2.24	0.52
29:4:541:PRO:O	29:4:545:GLN:N	2.39	0.52
32:A:1276:A:N6	32:A:1299:A:H62	2.08	0.52
7:F:126:TYR:O	7:F:134:GLN:NE2	2.42	0.52
30:a:143:THR:HG22	30:a:144:LEU:H	1.75	0.52
31:b:117:ALA:O	31:b:142:MET:N	2.43	0.52
22:X:86:ARG:NE	22:X:392:GLU:OE1	2.43	0.52
24:D:232:THR:N	24:D:236:GLY:O	2.43	0.52
9:I:181:ILE:HG12	26:Q:39:ILE:HG12	1.91	0.52
29:4:58:VAL:HG23	29:4:58:VAL:O	2.09	0.52
31:b:214:LEU:O	31:b:243:ARG:NH1	2.41	0.52
1:0:166:TYR:O	15:O:199:TRP:NE1	2.40	0.51
9:I:183:HIS:CG	32:A:1015:A:N9	2.78	0.51
10:J:70:PRO:HB3	10:J:117:ASP:HB3	1.91	0.51
30:a:122:VAL:CG2	30:a:152:MET:SD	2.98	0.51
13:M:20:ARG:NH2	13:M:42:PRO:O	2.44	0.51
8:H:149:THR:HG22	8:H:150:GLY:N	2.25	0.51
22:X:317:PHE:N	32:A:1374:A:OP1	2.38	0.51
26:Q:3:LYS:HD2	32:A:976:A:P	2.50	0.51
29:4:599:PHE:O	29:4:604:LYS:N	2.43	0.51
24:D:363:ALA:O	24:D:367:GLY:N	2.44	0.51
1:0:63:ARG:NH2	1:0:110:ASP:OD2	2.43	0.51
29:4:305:ILE:O	29:4:312:LYS:NZ	2.34	0.51
5:C:37:ASN:O	5:C:43:ARG:NH2	2.44	0.50
23:Y:313:PHE:HA	23:Y:314:PRO:C	2.36	0.50
9:I:187:ARG:HG3	26:Q:45:TYR:CD1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:165:LYS:NZ	32:A:1149:G:OP2	2.44	0.50
26:Q:53:GLN:HB3	32:A:1597:C:H42	1.76	0.50
29:4:402:GLY:HA2	29:4:441:THR:HG21	1.91	0.50
32:A:1179:G:H5'	32:A:1180:U:O5'	2.12	0.50
32:A:1211:G:N2	32:A:1354:A:H62	2.09	0.50
9:I:187:ARG:CZ	26:Q:45:TYR:CD2	2.95	0.50
30:a:146:ALA:O	30:a:150:ALA:N	2.45	0.50
32:A:936:G:HO2'	32:A:1107:U:HO2'	1.58	0.50
10:J:62:VAL:N	10:J:106:GLN:O	2.44	0.50
9:I:187:ARG:HG3	26:Q:45:TYR:CG	2.47	0.49
24:D:300:ARG:O	24:D:339:SER:OG	2.29	0.49
2:1:189:LYS:NZ	2:1:235:ASN:O	2.46	0.49
10:J:64:CYS:CB	10:J:81:CYS:SG	2.76	0.49
17:R:161:ILE:HG22	17:R:161:ILE:O	2.12	0.49
29:4:200:ASP:OD2	29:4:243:ASN:N	2.45	0.49
22:X:382:PHE:HD1	25:G:314:MET:HE2	1.77	0.49
9:I:183:HIS:HA	32:A:1015:A:C1'	2.42	0.49
1:0:135:MET:SD	1:0:135:MET:N	2.85	0.49
19:T:137:ARG:NE	40:T:301:HOH:O	2.41	0.49
2:1:211:ARG:HE	23:Y:359:SER:C	2.20	0.48
29:4:501:ASP:OD1	29:4:537:ARG:NH2	2.43	0.48
32:A:1400:U:O2'	32:A:1401:G:P	2.70	0.48
24:D:316:CYS:SG	24:D:334:ALA:N	2.86	0.48
32:A:817:G:N2	32:A:851:A:O2'	2.25	0.48
25:G:246:ARG:HA	25:G:246:ARG:HH11	1.78	0.48
31:b:195:ARG:HH12	31:b:206:THR:HG22	1.78	0.48
31:b:94:ASP:OD2	31:b:103:THR:OG1	2.31	0.48
32:A:1564:A:O2'	32:A:1565:A:O5'	2.27	0.48
25:G:258:GLU:O	25:G:259:PRO:C	2.55	0.48
17:R:317:ALA:O	17:R:321:ALA:N	2.47	0.48
22:X:210:TRP:CH2	22:X:242:ILE:HD12	2.48	0.48
25:G:286:TYR:O	25:G:326:HIS:ND1	2.43	0.48
29:4:481:LEU:O	29:4:485:ALA:N	2.43	0.48
32:A:688:A:HO2'	32:A:689:U:P	2.34	0.48
15:O:97:ARG:NH1	32:A:871:A:OP2	2.46	0.48
31:b:80:VAL:HG22	31:b:317:VAL:HG11	1.96	0.48
32:A:889:G:N2	32:A:902:G:OP1	2.47	0.48
22:X:169:LEU:O	22:X:179:ASP:N	2.46	0.47
5:C:58:ALA:HB1	5:C:59:PRO:CD	2.43	0.47
21:W:84:LEU:O	21:W:90:THR:OG1	2.32	0.47
25:G:118:GLU:OE1	32:A:1307:G:O2'	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:4:491:GLN:O	29:4:495:HIS:ND1	2.47	0.47
32:A:764:A:O2'	32:A:765:C:OP2	2.29	0.47
17:R:170:ARG:O	17:R:189:ARG:NH1	2.43	0.47
32:A:688:A:O2'	32:A:689:U:P	2.73	0.47
9:I:183:HIS:CG	32:A:1015:A:C8	3.03	0.47
10:J:66:PHE:CG	10:J:81:CYS:HA	2.50	0.47
29:4:191:LEU:HD23	29:4:247:ILE:HD13	1.96	0.47
30:a:296:LEU:HD23	30:a:298:GLY:N	2.30	0.47
32:A:1045:G:OP2	37:A:1702:SPM:H122	2.14	0.47
32:A:1443:U:O2'	32:A:1445:G:N7	2.39	0.47
25:G:139:GLN:OE1	25:G:139:GLN:N	2.48	0.47
1:0:19:ARG:NH1	32:A:808:C:OP1	2.48	0.47
2:1:199:CYS:O	2:1:203:ASP:N	2.48	0.47
9:I:181:ILE:HG12	26:Q:39:ILE:CG1	2.45	0.47
25:G:229:LEU:HD21	25:G:241:VAL:HG11	1.97	0.47
29:4:513:TRP:NE1	29:4:554:ASP:OD2	2.46	0.47
1:0:110:ASP:OD1	1:0:110:ASP:N	2.45	0.46
8:H:149:THR:HG22	8:H:150:GLY:H	1.80	0.46
9:I:185:GLY:C	32:A:1013:A:H1'	2.39	0.46
10:J:66:PHE:N	10:J:81:CYS:SG	2.88	0.46
22:X:192:LYS:NZ	22:X:227:GLU:OE1	2.48	0.46
30:a:143:THR:HG22	30:a:144:LEU:N	2.31	0.46
31:b:222:ILE:HG22	31:b:287:ALA:HB1	1.97	0.46
6:E:5:GLU:N	6:E:94:VAL:O	2.49	0.46
6:E:37:ARG:NH1	6:E:69:TYR:OH	2.48	0.46
32:A:1522:U:H3'	32:A:1523:A:H5''	1.98	0.46
8:H:123:SER:HB3	8:H:127:TYR:HB2	1.96	0.46
10:J:64:CYS:SG	10:J:82:ARG:HB3	2.54	0.46
22:X:242:ILE:HD11	35:X:502:GDP:N3	2.31	0.46
32:A:843:G:N2	32:A:846:A:OP2	2.46	0.46
5:C:144:SER:O	29:4:140:LEU:HD22	2.16	0.46
7:F:160:PRO:HB2	7:F:167:PHE:HB3	1.97	0.46
29:4:69:ALA:O	29:4:73:ALA:N	2.49	0.46
32:A:942:A:N6	32:A:1047:A:OP2	2.49	0.46
6:E:42:LEU:O	6:E:45:ARG:NH2	2.48	0.46
30:a:249:MET:N	30:a:249:MET:HE2	2.30	0.46
32:A:1479:C:O2'	32:A:1480:A:O4'	2.33	0.46
2:1:114:LEU:O	25:G:110:TYR:OH	2.26	0.46
4:B:239:ASN:ND2	4:B:242:SER:OG	2.49	0.46
12:L:86:ASP:OD1	12:L:87:ASP:N	2.49	0.46
31:b:93:LEU:HD23	31:b:166:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:120:ARG:NH1	31:b:298:GLU:OE1	2.49	0.46
32:A:878:G:O6	32:A:896:A:N6	2.49	0.46
9:I:183:HIS:CD2	32:A:1015:A:N3	2.84	0.46
9:I:187:ARG:NH1	26:Q:45:TYR:CD2	2.84	0.46
32:A:734:C:N3	32:A:739:C:N4	2.64	0.46
32:A:1108:C:H4'	32:A:1109:A:OP2	2.14	0.46
9:I:162:MET:SD	26:Q:19:VAL:CG1	3.04	0.46
20:U:173:LEU:O	20:U:177:VAL:HG23	2.16	0.46
22:X:132:THR:OG1	22:X:134:LYS:NZ	2.48	0.46
25:G:241:VAL:O	25:G:245:ARG:N	2.49	0.45
28:Z:54:ASN:ND2	28:Z:57:THR:OG1	2.49	0.45
7:F:162:LEU:O	7:F:162:LEU:HD12	2.16	0.45
10:J:80:CYS:C	10:J:93:CYS:SG	2.99	0.45
25:G:138:ILE:HD11	25:G:140:TRP:CE2	2.52	0.45
32:A:764:A:O2'	32:A:765:C:P	2.74	0.45
12:L:224:ARG:HA	12:L:227:LEU:HB2	1.98	0.45
26:Q:61:ARG:HG3	32:A:1599:A:H5'	1.98	0.45
13:M:67:ALA:HB2	17:R:196:TYR:CE1	2.52	0.45
15:O:92:LYS:NZ	32:A:919:A:OP1	2.33	0.45
18:S:83:ARG:NH1	18:S:93:LYS:O	2.50	0.45
30:a:296:LEU:HD23	30:a:297:SER:N	2.32	0.45
25:G:237:GLU:OE1	25:G:237:GLU:N	2.50	0.45
18:S:111:GLU:OE2	18:S:117:LEU:N	2.50	0.45
25:G:220:GLN:NE2	32:A:1293:C:OP2	2.48	0.45
30:a:97:ASN:C	30:a:99:LEU:N	2.72	0.45
29:4:501:ASP:OD2	29:4:537:ARG:NH1	2.49	0.45
21:W:102:GLY:O	21:W:140:VAL:N	2.45	0.45
23:Y:313:PHE:HB3	23:Y:314:PRO:HA	1.98	0.45
27:V:270:PRO:O	27:V:346:LYS:NZ	2.49	0.45
32:A:1119:U:H2'	32:A:1120:C:O4'	2.16	0.45
8:H:71:ILE:O	8:H:150:GLY:N	2.50	0.44
15:O:105:CYS:HB2	15:O:142:VAL:HA	1.99	0.44
22:X:138:LEU:HD21	22:X:261:ALA:HB1	1.99	0.44
29:4:508:VAL:HG12	29:4:508:VAL:O	2.17	0.44
30:a:97:ASN:O	30:a:98:GLY:C	2.59	0.44
32:A:1176:G:H21	32:A:1483:C:H5	1.64	0.44
2:1:255:ASN:N	2:1:259:GLU:OE1	2.47	0.44
11:K:80:ARG:NH2	32:A:1350:G:OP1	2.50	0.44
12:L:218:GLN:O	12:L:222:LYS:N	2.47	0.44
8:H:132:VAL:HG13	11:K:125:ARG:HH12	1.82	0.44
10:J:64:CYS:CB	10:J:81:CYS:HB3	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:G:78:ILE:HG22	25:G:78:ILE:O	2.17	0.44
29:4:120:ILE:HG22	29:4:120:ILE:O	2.18	0.44
32:A:1383:A:N3	32:A:1383:A:H2'	2.33	0.44
22:X:242:ILE:HD11	35:X:502:GDP:C2	2.53	0.44
22:X:383:LEU:HD22	25:G:314:MET:HE1	2.00	0.44
23:Y:312:GLU:HG2	29:4:67:LYS:HD2	1.99	0.44
26:Q:10:ARG:HD2	26:Q:30:LEU:HD21	2.00	0.44
23:Y:334:LEU:HD23	23:Y:334:LEU:H	1.82	0.44
25:G:379:ARG:NH1	25:G:380:LYS:O	2.51	0.44
32:A:1256:A:C6	32:A:1338:A:N1	2.85	0.44
4:B:108:GLY:O	4:B:115:ILE:N	2.43	0.44
10:J:80:CYS:O	10:J:81:CYS:HB2	2.18	0.44
25:G:258:GLU:HB2	25:G:270:SER:HB2	2.00	0.44
25:G:268:ALA:O	25:G:287:LYS:N	2.43	0.44
31:b:382:VAL:HG21	31:b:400:LYS:HE3	1.99	0.44
10:J:93:CYS:SG	10:J:93:CYS:O	2.75	0.43
12:L:206:LYS:NZ	32:A:762:G:OP1	2.37	0.43
32:A:1214:A:N1	32:A:1351:G:O2'	2.49	0.43
28:Z:40:LEU:HD21	28:Z:44:LYS:HB3	1.98	0.43
32:A:1562:G:O2'	32:A:1563:U:P	2.76	0.43
1:O:103:ASP:OD1	1:O:105:THR:OG1	2.32	0.43
5:C:58:ALA:HB1	5:C:59:PRO:HD2	2.00	0.43
7:F:171:PRO:HB3	7:F:230:ALA:HB1	2.00	0.43
8:H:117:ARG:NE	8:H:135:GLU:OE1	2.50	0.43
11:K:51:ARG:NH2	32:A:1402:A:O5'	2.52	0.43
2:1:66:TRP:O	2:1:69:VAL:N	2.50	0.43
2:1:211:ARG:O	2:1:211:ARG:NH1	2.41	0.43
4:B:197:HIS:NE2	4:B:240:ASP:O	2.50	0.43
22:X:365:TRP:NE1	22:X:395:CYS:O	2.52	0.43
31:b:376:GLU:O	31:b:405:ILE:N	2.50	0.43
9:I:188:PRO:HG3	26:Q:42:ARG:HD3	2.00	0.43
15:O:105:CYS:SG	15:O:108:CYS:CB	3.07	0.43
17:R:136:VAL:O	17:R:186:TRP:NE1	2.43	0.43
4:B:188:ARG:NH2	4:B:191:ASP:OD2	2.50	0.43
10:J:78:ARG:NH2	10:J:117:ASP:OD2	2.51	0.43
20:U:64:ARG:NH1	32:A:844:A:O2'	2.51	0.43
23:Y:314:PRO:O	23:Y:315:ILE:C	2.62	0.43
24:D:189:ARG:NE	30:a:303:ASP:O	2.52	0.43
24:D:196:ASN:ND2	30:a:300:GLU:OE2	2.51	0.43
32:A:1564:A:C2'	32:A:1565:A:O5'	2.66	0.43
19:T:4:LYS:O	19:T:11:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:1133:C:N3	32:A:1133:C:N1	2.64	0.43
22:X:242:ILE:HD11	35:X:502:GDP:C4	2.54	0.43
24:D:232:THR:OG1	24:D:236:GLY:N	2.52	0.43
30:a:122:VAL:HG11	30:a:140:TRP:HE3	1.82	0.43
11:K:29:TYR:CE2	11:K:38:VAL:HG21	2.53	0.43
5:C:76:LEU:HD22	8:H:138:THR:HG23	2.01	0.42
7:F:171:PRO:HB2	30:a:193:LEU:HD22	2.01	0.42
30:a:92:ARG:HA	30:a:95:ALA:HB3	2.01	0.42
14:N:93:ASP:O	14:N:97:GLY:N	2.41	0.42
23:Y:338:LEU:HD11	23:Y:355:THR:HG21	2.01	0.42
13:M:55:ASP:OD2	19:T:146:GLN:NE2	2.52	0.42
32:A:1318:A:H3'	32:A:1319:A:H5''	2.01	0.42
32:A:1420:U:O4'	32:A:1421:G:N2	2.52	0.42
2:1:131:THR:OG1	8:H:149:THR:HG21	2.19	0.42
27:V:314:VAL:HG22	27:V:316:GLN:H	1.83	0.42
32:A:945:G:O6	37:A:1702:SPM:H21	2.19	0.42
2:1:163:VAL:HG23	23:Y:315:ILE:HD11	2.02	0.42
25:G:138:ILE:HD11	25:G:140:TRP:CZ2	2.54	0.42
26:Q:45:TYR:CZ	26:Q:46:GLU:O	2.72	0.42
32:A:1482:A:O5'	32:A:1483:C:P	2.77	0.42
8:H:184:ILE:O	8:H:184:ILE:HG22	2.20	0.42
18:S:42:ARG:NH1	18:S:43:GLU:O	2.52	0.42
22:X:379:GLU:O	22:X:383:LEU:HD23	2.19	0.42
2:1:118:ALA:O	2:1:122:HIS:N	2.48	0.42
5:C:58:ALA:HB3	5:C:60:HIS:CE1	2.54	0.42
29:4:450:PRO:O	29:4:454:ARG:N	2.49	0.42
30:a:304:ASP:O	30:a:305:LEU:C	2.61	0.42
9:I:183:HIS:NE2	32:A:1015:A:C2	2.88	0.42
25:G:198:ARG:O	25:G:246:ARG:N	2.53	0.42
32:A:1417:A:H2'	32:A:1418:G:C8	2.54	0.42
32:A:1599:A:H1'	32:A:1600:A:C5	2.54	0.42
9:I:183:HIS:ND1	32:A:1015:A:C5	2.88	0.42
29:4:396:ILE:HG22	29:4:400:LEU:HD12	2.02	0.42
10:J:91:ALA:HB1	10:J:123:LEU:HD12	2.02	0.41
19:T:160:ARG:NH2	32:A:683:G:OP1	2.53	0.41
32:A:1383:A:H2'	32:A:1384:A:H5'	2.02	0.41
32:A:1492:A:H3'	32:A:1493:C:C5'	2.50	0.41
7:F:71:THR:HA	25:G:251:GLU:HG3	2.02	0.41
9:I:183:HIS:NE2	32:A:1015:A:N3	2.68	0.41
11:K:111:PHE:HZ	11:K:123:ILE:HD13	1.85	0.41
30:a:99:LEU:HD23	30:a:100:LEU:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:A:1596:A:H3'	32:A:1597:C:H5''	2.02	0.41
8:H:120:LEU:HD21	11:K:101:LYS:NZ	2.34	0.41
9:I:187:ARG:HG2	26:Q:45:TYR:CB	2.49	0.41
28:Z:75:HIS:NE2	32:A:1335:U:OP1	2.51	0.41
30:a:250:GLU:O	30:a:251:TYR:C	2.62	0.41
12:L:128:ARG:NH1	32:A:1042:U:OP1	2.54	0.41
27:V:123:ASP:OD1	27:V:123:ASP:N	2.53	0.41
30:a:100:LEU:HD11	30:a:129:LEU:HD11	2.03	0.41
8:H:50:LEU:HD23	29:4:82:THR:HG22	2.01	0.41
25:G:309:ASP:O	25:G:313:LEU:HD23	2.20	0.41
27:V:110:HIS:NE2	27:V:375:TYR:OH	2.53	0.41
32:A:1465:C:H2'	32:A:1466:C:H1'	2.03	0.41
8:H:120:LEU:HD21	11:K:101:LYS:HZ2	1.85	0.41
11:K:57:LEU:HD23	23:Y:350:PHE:CZ	2.56	0.41
32:A:1297:G:H2'	32:A:1298:U:H5'	2.01	0.41
32:A:1299:A:H3'	32:A:1300:A:H5''	2.02	0.41
32:A:1412:G:H2'	32:A:1413:U:H5'	2.02	0.41
7:F:42:LYS:N	7:F:73:LEU:O	2.46	0.41
9:I:151:VAL:O	9:I:178:ASN:N	2.50	0.41
21:W:87:SER:OG	21:W:90:THR:OG1	2.34	0.41
22:X:121:ALA:N	22:X:301:TRP:O	2.53	0.41
27:V:285:ALA:O	27:V:289:ALA:N	2.51	0.41
30:a:122:VAL:HG21	30:a:152:MET:SD	2.61	0.41
22:X:177:ARG:HG3	22:X:178:PHE:H	1.85	0.41
32:A:1462:G:H2'	32:A:1463:G:C8	2.56	0.41
32:A:1506:U:H5	32:A:1539:C:H42	1.69	0.41
32:A:1540:A:H5''	32:A:1541:U:OP2	2.20	0.41
2:1:81:VAL:O	2:1:99:LYS:NZ	2.54	0.41
4:B:89:VAL:O	4:B:89:VAL:HG12	2.21	0.41
7:F:70:LYS:HG2	25:G:253:LYS:HE3	2.03	0.41
9:I:94:ASN:ND2	32:A:989:U:OP1	2.54	0.41
9:I:185:GLY:HA2	32:A:1013:A:H1'	2.00	0.41
12:L:212:ARG:NH2	12:L:216:GLU:OE2	2.53	0.41
12:L:224:ARG:HA	12:L:227:LEU:HD12	2.02	0.41
15:O:94:CYS:HB2	15:O:108:CYS:SG	2.61	0.41
15:O:137:ALA:HB3	15:O:138:PRO:HD3	2.03	0.41
15:O:185:SER:O	17:R:183:LYS:NZ	2.53	0.41
25:G:134:ARG:O	25:G:134:ARG:HG2	2.21	0.41
28:Z:40:LEU:HG	28:Z:44:LYS:HB2	2.03	0.41
30:a:92:ARG:N	30:a:92:ARG:CD	2.83	0.41
32:A:1600:A:N3	32:A:1600:A:H2'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:105:CYS:HB3	16:P:68:CYS:HG	1.61	0.41
7:F:158:LEU:HD22	7:F:233:ASN:HD22	1.85	0.41
15:O:63:GLU:OE1	15:O:112:LYS:NZ	2.53	0.41
32:A:812:A:O2'	32:A:814:A:N1	2.44	0.41
24:D:313:GLY:N	24:D:331:ASP:OD1	2.51	0.40
27:V:265:LYS:O	27:V:269:SER:N	2.51	0.40
32:A:1388:C:H2'	32:A:1389:G:H5'	2.03	0.40
15:O:94:CYS:SG	15:O:105:CYS:SG	3.19	0.40
22:X:276:ARG:NH2	22:X:286:GLU:OE1	2.54	0.40
23:Y:342:PRO:HG3	23:Y:394:PHE:HA	2.02	0.40
29:4:102:GLU:O	29:4:106:PHE:N	2.53	0.40
31:b:195:ARG:NH1	31:b:206:THR:HG22	2.36	0.40
32:A:1260:A:C6	32:A:1336:G:C5	3.09	0.40
32:A:1365:A:H1'	32:A:1419:G:H2'	2.03	0.40
11:K:63:LEU:HD13	11:K:67:LEU:HD22	2.03	0.40
14:N:88:VAL:O	14:N:88:VAL:HG13	2.21	0.40
15:O:105:CYS:SG	15:O:108:CYS:N	2.94	0.40
6:E:113:LEU:HD22	26:Q:67:GLU:OE2	2.21	0.40
21:W:129:VAL:HG23	21:W:130:ASP:N	2.37	0.40
32:A:1188:A:H5'	32:A:1189:U:O5'	2.22	0.40
32:A:1366:C:H2'	32:A:1369:U:H1'	2.04	0.40
24:D:290:ILE:HD12	24:D:292:HIS:O	2.22	0.40
24:D:299:LYS:HG3	24:D:299:LYS:O	2.22	0.40
32:A:976:A:C2	32:A:977:A:C4	3.10	0.40
32:A:1385:C:H2'	32:A:1386:U:H3'	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	0	208/218 (95%)	199 (96%)	9 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	274/323 (85%)	267 (97%)	7 (3%)	0	100	100
3	3	68/199 (34%)	67 (98%)	1 (2%)	0	100	100
4	B	223/296 (75%)	214 (96%)	9 (4%)	0	100	100
5	C	130/167 (78%)	127 (98%)	3 (2%)	0	100	100
6	E	113/125 (90%)	111 (98%)	2 (2%)	0	100	100
7	F	198/242 (82%)	193 (98%)	5 (2%)	0	100	100
8	H	138/201 (69%)	132 (96%)	6 (4%)	0	100	100
9	I	131/194 (68%)	125 (95%)	6 (5%)	0	100	100
10	J	106/138 (77%)	96 (91%)	9 (8%)	1 (1%)	14	43
11	K	99/128 (77%)	95 (96%)	4 (4%)	0	100	100
12	L	172/257 (67%)	165 (96%)	7 (4%)	0	100	100
13	M	117/137 (85%)	116 (99%)	1 (1%)	0	100	100
14	N	108/130 (83%)	102 (94%)	6 (6%)	0	100	100
15	O	192/258 (74%)	184 (96%)	8 (4%)	0	100	100
16	P	95/142 (67%)	90 (95%)	5 (5%)	0	100	100
17	R	293/360 (81%)	285 (97%)	8 (3%)	0	100	100
18	S	133/190 (70%)	130 (98%)	3 (2%)	0	100	100
19	T	166/173 (96%)	165 (99%)	0	1 (1%)	21	51
20	U	174/205 (85%)	171 (98%)	3 (2%)	0	100	100
21	W	98/187 (52%)	96 (98%)	2 (2%)	0	100	100
22	X	350/398 (88%)	340 (97%)	10 (3%)	0	100	100
23	Y	119/395 (30%)	116 (98%)	3 (2%)	0	100	100
24	D	316/430 (74%)	308 (98%)	8 (2%)	0	100	100
25	G	306/396 (77%)	296 (97%)	10 (3%)	0	100	100
26	Q	81/87 (93%)	76 (94%)	4 (5%)	1 (1%)	10	38
27	V	348/414 (84%)	340 (98%)	8 (2%)	0	100	100
28	Z	81/106 (76%)	79 (98%)	2 (2%)	0	100	100
29	4	584/689 (85%)	568 (97%)	15 (3%)	1 (0%)	43	71
30	a	147/343 (43%)	138 (94%)	9 (6%)	0	100	100
31	b	315/407 (77%)	301 (96%)	14 (4%)	0	100	100
All	All	5883/7935 (74%)	5692 (97%)	187 (3%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	81	CYS
26	Q	3	LYS
19	T	151	SER
29	4	385	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	184/190 (97%)	184 (100%)	0	100	100
2	1	254/291 (87%)	254 (100%)	0	100	100
3	3	65/166 (39%)	65 (100%)	0	100	100
4	B	198/249 (80%)	198 (100%)	0	100	100
5	C	115/143 (80%)	115 (100%)	0	100	100
6	E	97/107 (91%)	97 (100%)	0	100	100
7	F	179/209 (86%)	178 (99%)	1 (1%)	78	77
8	H	130/180 (72%)	130 (100%)	0	100	100
9	I	101/146 (69%)	101 (100%)	0	100	100
10	J	93/118 (79%)	93 (100%)	0	100	100
11	K	91/113 (80%)	91 (100%)	0	100	100
12	L	158/226 (70%)	158 (100%)	0	100	100
13	M	97/113 (86%)	97 (100%)	0	100	100
14	N	96/115 (84%)	96 (100%)	0	100	100
15	O	175/230 (76%)	175 (100%)	0	100	100
16	P	88/123 (72%)	88 (100%)	0	100	100
17	R	264/318 (83%)	264 (100%)	0	100	100
18	S	116/164 (71%)	116 (100%)	0	100	100
19	T	153/157 (98%)	153 (100%)	0	100	100
20	U	152/174 (87%)	152 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	W	87/158 (55%)	87 (100%)	0	100	100
22	X	311/351 (89%)	311 (100%)	0	100	100
23	Y	112/357 (31%)	112 (100%)	0	100	100
24	D	272/357 (76%)	272 (100%)	0	100	100
25	G	270/342 (79%)	266 (98%)	4 (2%)	57	66
26	Q	75/78 (96%)	75 (100%)	0	100	100
27	V	317/364 (87%)	317 (100%)	0	100	100
28	Z	79/95 (83%)	79 (100%)	0	100	100
29	4	526/609 (86%)	526 (100%)	0	100	100
30	a	133/288 (46%)	133 (100%)	0	100	100
31	b	269/350 (77%)	269 (100%)	0	100	100
All	All	5257/6881 (76%)	5252 (100%)	5 (0%)	87	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	F	161	ILE
25	G	246	ARG
25	G	251	GLU
25	G	255	GLN
25	G	280	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	145	HIS
2	1	185	HIS
4	B	167	HIS
6	E	54	HIS
7	F	233	ASN
8	H	122	GLN
10	J	105	HIS
11	K	119	GLN
13	M	75	HIS
15	O	130	HIS
15	O	147	HIS
15	O	169	GLN

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Mol	Chain	Res	Type
15	O	223	HIS
18	S	66	HIS
19	T	85	GLN
22	X	69	ASN
22	X	73	GLN
22	X	235	ASN
22	X	302	HIS
23	Y	337	HIS
23	Y	378	ASN
24	D	127	ASN
26	Q	79	ASN
27	V	122	GLN
27	V	188	HIS
28	Z	54	ASN
29	4	295	ASN
29	4	326	GLN
29	4	373	HIS
29	4	398	ASN
29	4	444	ASN
29	4	470	GLN
31	b	90	GLN
31	b	253	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	A	944/954 (98%)	242 (25%)	7 (0%)

All (242) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
32	A	650	U
32	A	651	A
32	A	680	U
32	A	688	A
32	A	689	U
32	A	695	A
32	A	697	G
32	A	704	U
32	A	705	C
32	A	713	C

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Mol	Chain	Res	Type
32	A	718	A
32	A	721	U
32	A	723	A
32	A	737	C
32	A	740	G
32	A	753	A
32	A	757	A
32	A	761	A
32	A	764	A
32	A	765	C
32	A	766	G
32	A	777	G
32	A	791	G
32	A	793	C
32	A	794	U
32	A	796	G
32	A	806	C
32	A	808	C
32	A	814	A
32	A	815	C
32	A	817	G
32	A	828	C
32	A	830	U
32	A	832	U
32	A	835	C
32	A	860	A
32	A	861	U
32	A	868	C
32	A	869	C
32	A	870	C
32	A	871	A
32	A	881	A
32	A	890	C
32	A	902	G
32	A	904	C
32	A	905	A
32	A	907	A
32	A	908	C
32	A	919	A
32	A	923	A
32	A	929	A
32	A	931	C

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Mol	Chain	Res	Type
32	A	938	A
32	A	939	A
32	A	940	A
32	A	941	G
32	A	942	A
32	A	943	G
32	A	950	A
32	A	954	C
32	A	955	A
32	A	958	C
32	A	961	U
32	A	962	C
32	A	963	C
32	A	964	C
32	A	967	A
32	A	975	A
32	A	978	A
32	A	985	U
32	A	986	G
32	A	991	G
32	A	992	U
32	A	993	A
32	A	994	A
32	A	1001	C
32	A	1002	C
32	A	1003	A
32	A	1004	G
32	A	1010	A
32	A	1011	C
32	A	1028	G
32	A	1042	U
32	A	1047	A
32	A	1049	A
32	A	1058	C
32	A	1065	C
32	A	1069	A
32	A	1073	G
32	A	1080	A
32	A	1081	U
32	A	1082	A
32	A	1094	U
32	A	1103	A

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Mol	Chain	Res	Type
32	A	1105	C
32	A	1106	C
32	A	1107	U
32	A	1115	U
32	A	1119	U
32	A	1121	A
32	A	1126	A
32	A	1137	A
32	A	1144	U
32	A	1151	C
32	A	1153	C
32	A	1155	G
32	A	1160	A
32	A	1167	A
32	A	1172	C
32	A	1174	U
32	A	1180	U
32	A	1182	C
32	A	1183	U
32	A	1184	U
32	A	1185	C
32	A	1186	A
32	A	1187	U
32	A	1189	U
32	A	1190	C
32	A	1192	C
32	A	1194	C
32	A	1201	A
32	A	1206	G
32	A	1212	U
32	A	1213	A
32	A	1214	A
32	A	1215	U
32	A	1222	A
32	A	1223	C
32	A	1226	C
32	A	1227	G
32	A	1229	U
32	A	1240	A
32	A	1248	C
32	A	1251	A
32	A	1254	C

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Mol	Chain	Res	Type
32	A	1269	U
32	A	1272	A
32	A	1273	G
32	A	1278	C
32	A	1283	A
32	A	1284	U
32	A	1285	G
32	A	1290	C
32	A	1292	A
32	A	1297	G
32	A	1298	U
32	A	1300	A
32	A	1317	A
32	A	1318	A
32	A	1319	A
32	A	1325	U
32	A	1326	A
32	A	1327	G
32	A	1328	G
32	A	1330	C
32	A	1331	A
32	A	1341	C
32	A	1343	A
32	A	1353	A
32	A	1357	A
32	A	1358	A
32	A	1359	U
32	A	1365	A
32	A	1366	C
32	A	1382	A
32	A	1384	A
32	A	1385	C
32	A	1386	U
32	A	1387	A
32	A	1388	C
32	A	1400	U
32	A	1401	G
32	A	1402	A
32	A	1405	C
32	A	1412	G
32	A	1414	C
32	A	1417	A

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Mol	Chain	Res	Type
32	A	1420	U
32	A	1421	G
32	A	1422	G
32	A	1426	U
32	A	1430	A
32	A	1442	G
32	A	1446	A
32	A	1448	U
32	A	1456	U
32	A	1461	A
32	A	1464	G
32	A	1466	C
32	A	1467	C
32	A	1468	U
32	A	1470	A
32	A	1474	G
32	A	1478	A
32	A	1480	A
32	A	1481	C
32	A	1482	A
32	A	1483	C
32	A	1484	C
32	A	1485	G
32	A	1492	A
32	A	1493	C
32	A	1495	C
32	A	1503	G
32	A	1512	A
32	A	1518	C
32	A	1519	A
32	A	1520	U
32	A	1521	U
32	A	1522	U
32	A	1523	A
32	A	1524	A
32	A	1525	C
32	A	1526	U
32	A	1527	A
32	A	1530	A
32	A	1531	C
32	A	1533	C
32	A	1536	A

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Mol	Chain	Res	Type
32	A	1538	G
32	A	1539	C
32	A	1540	A
32	A	1541	U
32	A	1546	A
32	A	1548	A
32	A	1549	G
32	A	1557	A
32	A	1563	U
32	A	1564	A
32	A	1565	A
32	A	1568	U
32	A	1569	G
32	A	1571	U
32	A	1572	A
32	A	1574	G
32	A	1582	G
32	A	1594	G
32	A	1595	G
32	A	1597	C
32	A	1598	G
32	A	1599	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	A	1046	A
32	A	1179	G
32	A	1214	A
32	A	1330	C
32	A	1386	U
32	A	1400	U
32	A	1597	C

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	B8T	A	1486	32	19,22,23	3.33	8 (42%)	26,31,34	0.84	1 (3%)
32	5MU	A	1076	32	19,22,23	0.40	0	28,32,35	0.51	0
9	5F0	I	184	9	8,8,9	0.56	0	7,9,11	1.21	1 (14%)
32	MA6	A	1584	32	23,26,27	1.28	3 (13%)	34,38,41	3.13	12 (35%)
32	5MC	A	1488	32	18,22,23	0.52	0	26,32,35	0.49	0
32	MA6	A	1583	32	23,26,27	1.27	3 (13%)	34,38,41	3.15	12 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	B8T	A	1486	32	-	0/7/27/28	0/2/2/2
32	5MU	A	1076	32	-	0/7/25/26	0/2/2/2
9	5F0	I	184	9	-	2/9/9/10	-
32	MA6	A	1584	32	-	2/11/29/30	0/3/3/3
32	5MC	A	1488	32	-	0/7/25/26	0/2/2/2
32	MA6	A	1583	32	-	1/11/29/30	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	1486	B8T	C4-N3	7.72	1.46	1.32
32	A	1486	B8T	C2-N3	6.02	1.48	1.36
32	A	1486	B8T	C6-C5	5.93	1.48	1.35
32	A	1486	B8T	C4-N4	4.87	1.45	1.35
32	A	1486	B8T	C2-N1	4.63	1.50	1.40
32	A	1486	B8T	C5-C4	3.55	1.48	1.40
32	A	1486	B8T	C6-N1	3.49	1.46	1.38
32	A	1584	MA6	C6-N6	3.41	1.46	1.36
32	A	1583	MA6	C6-N6	3.37	1.46	1.36
32	A	1486	B8T	O2-C2	-2.92	1.18	1.23
32	A	1583	MA6	C5-C4	-2.57	1.34	1.39
32	A	1584	MA6	C5-C4	-2.50	1.34	1.39
32	A	1584	MA6	C5-N7	-2.31	1.34	1.39
32	A	1583	MA6	C5-N7	-2.25	1.34	1.39

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	1583	MA6	N1-C6-N6	-12.26	103.68	117.08
32	A	1584	MA6	N1-C6-N6	-12.18	103.76	117.08
32	A	1584	MA6	C5-C6-N6	6.18	136.07	125.30
32	A	1583	MA6	C5-C6-N6	6.16	136.03	125.30
32	A	1583	MA6	N1-C2-N3	-5.43	120.11	128.60
32	A	1584	MA6	N1-C2-N3	-5.37	120.19	128.60
32	A	1583	MA6	C5-C4-N3	-5.24	119.91	126.75
32	A	1584	MA6	C5-C4-N3	-5.23	119.92	126.75
32	A	1583	MA6	N9-C8-N7	-4.28	108.06	113.91
32	A	1584	MA6	N9-C8-N7	-4.19	108.18	113.91
32	A	1584	MA6	C4-C5-C6	3.61	119.92	115.88
32	A	1583	MA6	C4-C5-C6	3.54	119.84	115.88
32	A	1583	MA6	C2-N3-C4	3.50	120.03	111.75
32	A	1584	MA6	C2-N3-C4	3.47	119.95	111.75
32	A	1584	MA6	C2-N1-C6	3.43	119.84	111.75
32	A	1583	MA6	C2-N1-C6	3.41	119.81	111.75
32	A	1583	MA6	N3-C4-N9	3.16	132.29	127.08
32	A	1584	MA6	N3-C4-N9	3.14	132.26	127.08
32	A	1583	MA6	C5-N7-C8	3.09	107.89	103.51
32	A	1584	MA6	C5-N7-C8	3.07	107.87	103.51
9	I	184	5F0	O-C-CB	-2.78	117.34	125.43
32	A	1486	B8T	C6-C5-C4	2.48	120.00	116.96
32	A	1583	MA6	C4-N9-C8	2.19	108.11	105.73
32	A	1584	MA6	C4-N9-C8	2.08	107.99	105.73
32	A	1583	MA6	C4-C5-N7	-2.04	108.14	110.62
32	A	1584	MA6	C4-C5-N7	-2.03	108.14	110.62

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	1584	MA6	C3'-C4'-C5'-O5'
32	A	1584	MA6	O4'-C4'-C5'-O5'
9	I	184	5F0	OD1-C1-CA-CB
32	A	1583	MA6	O4'-C4'-C5'-O5'
9	I	184	5F0	O-C-CB-CA

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	A	1584	MA6	2	0
32	A	1583	MA6	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 19 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	FES	P	201	16,6	0,4,4	-	-	-	-	-
33	FES	T	201	19,13	0,4,4	-	-	-	-	-
35	GDP	X	502	-	28,30,30	0.49	0	44,47,47	0.50	0
36	NAD	A	1701	38	45,48,48	0.72	1 (2%)	63,73,73	0.70	1 (1%)
34	ATP	X	501	-	29,33,33	0.52	0	44,52,52	0.79	1 (2%)
37	SPM	A	1702	-	13,13,13	0.35	0	12,12,12	0.95	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	FES	P	201	16,6	-	-	0/1/1/1
33	FES	T	201	19,13	-	-	0/1/1/1
35	GDP	X	502	-	-	2/16/32/32	0/3/3/3
36	NAD	A	1701	38	-	4/30/62/62	0/5/5/5
34	ATP	X	501	-	-	2/22/38/38	0/3/3/3
37	SPM	A	1702	-	-	1/11/11/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	A	1701	NAD	O4D-C1D	-2.28	1.37	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	1701	NAD	PN-O3-PA	-2.22	125.20	132.83
34	X	501	ATP	PA-O3A-PB	-2.11	125.58	132.83

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	X	501	ATP	C5'-O5'-PA-O1A
37	A	1702	SPM	N10-C11-C12-C13
35	X	502	GDP	O4'-C4'-C5'-O5'
35	X	502	GDP	C3'-C4'-C5'-O5'
34	X	501	ATP	C5'-O5'-PA-O3A
36	A	1701	NAD	C5B-O5B-PA-O3
36	A	1701	NAD	PA-O3-PN-O2N
36	A	1701	NAD	C5B-O5B-PA-O1A
36	A	1701	NAD	C4B-C5B-O5B-PA

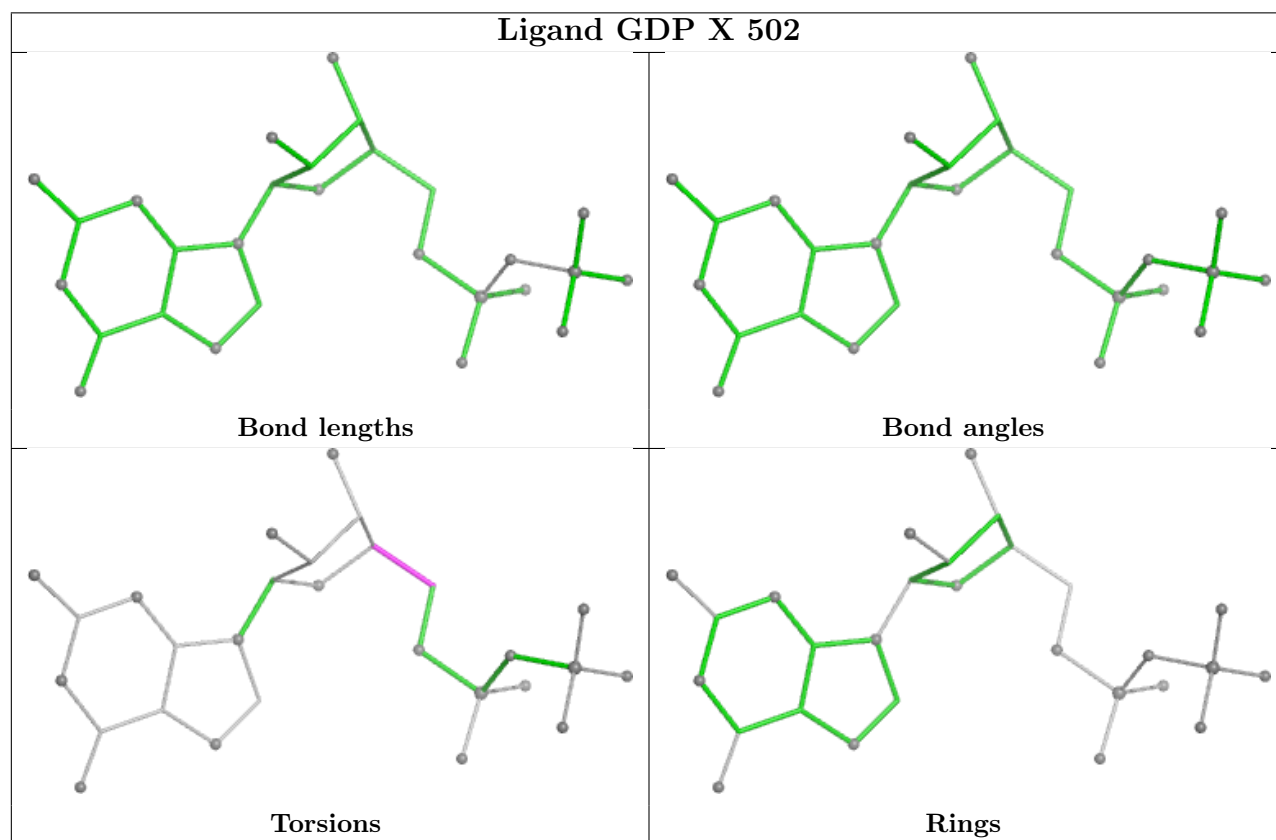
There are no ring outliers.

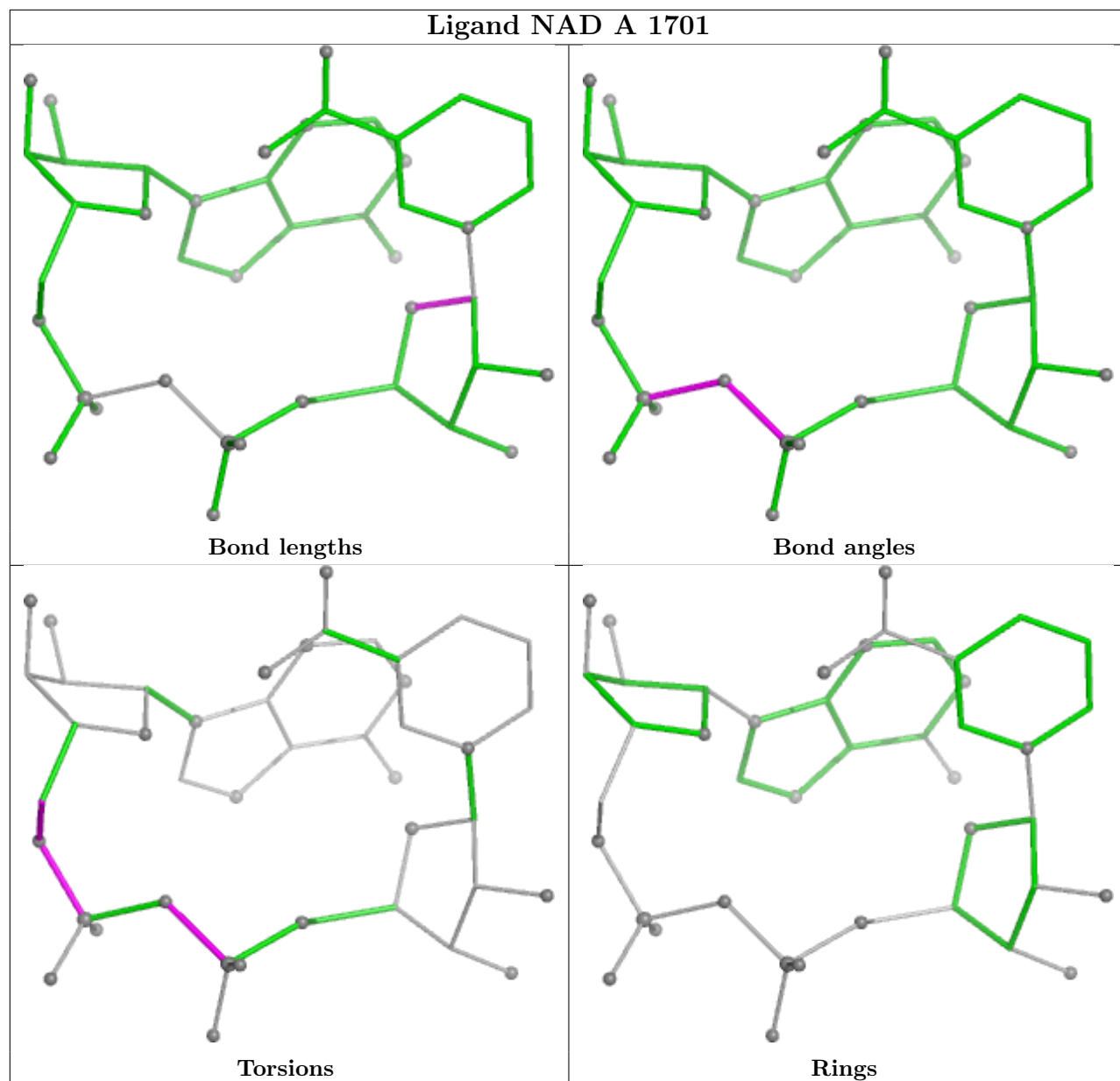
5 monomers are involved in 14 short contacts:

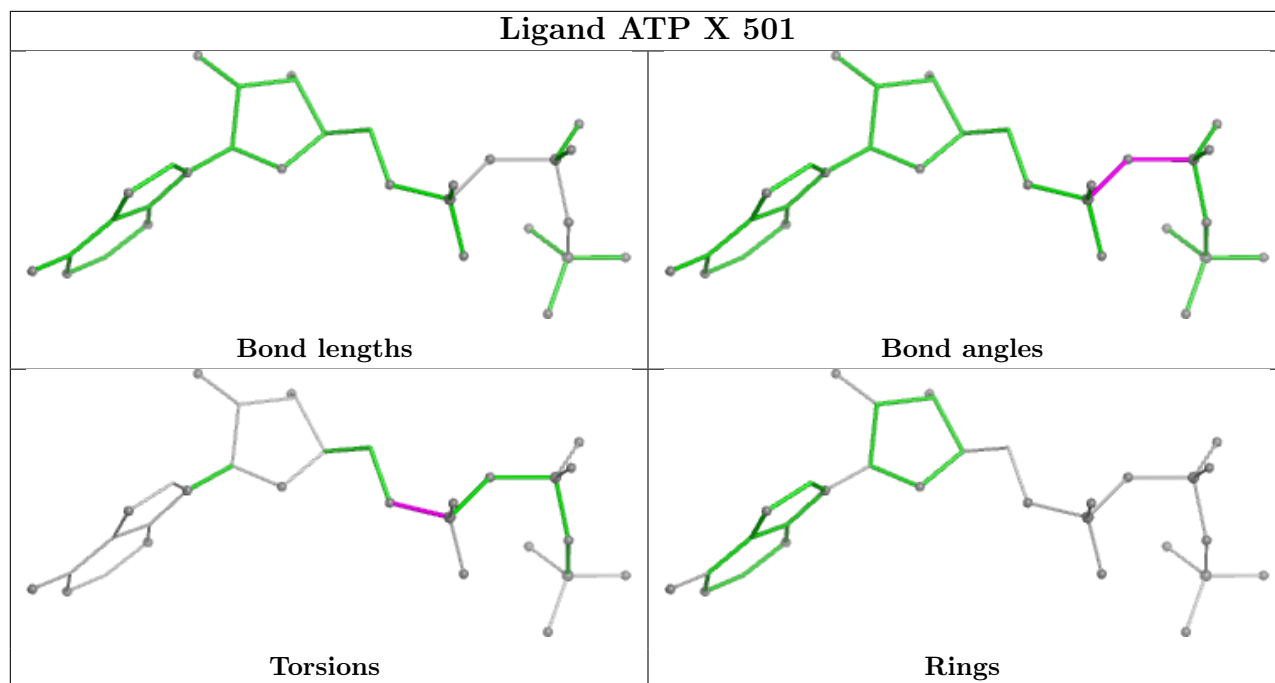
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	P	201	FES	4	0
33	T	201	FES	1	0
35	X	502	GDP	5	0
34	X	501	ATP	1	0
37	A	1702	SPM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1486:B8T	O3'	1487:C	P	4.83
1	A	1485:G	O3'	1486:B8T	P	3.56

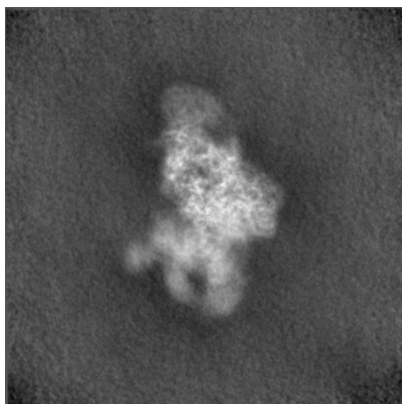
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54129. These allow visual inspection of the internal detail of the map and identification of artifacts.

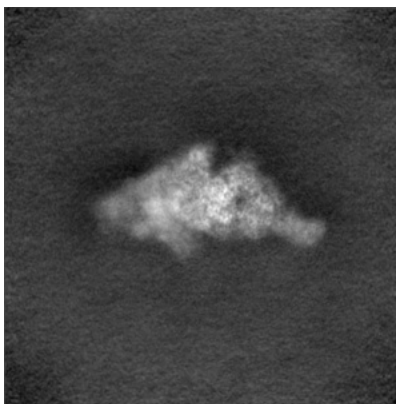
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

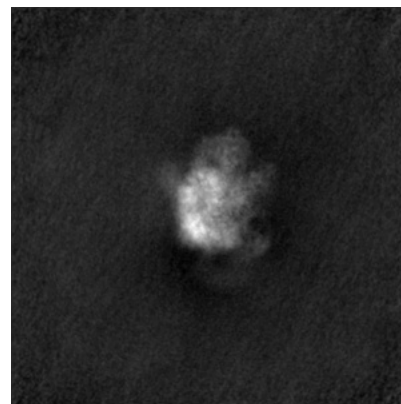
6.1.1 Primary map



X

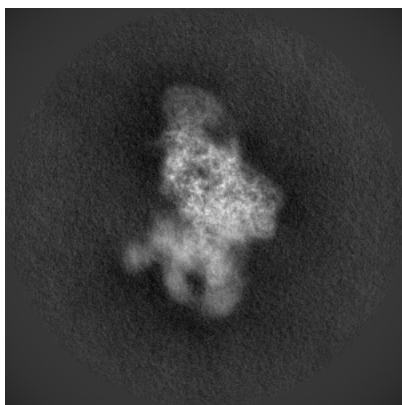


Y

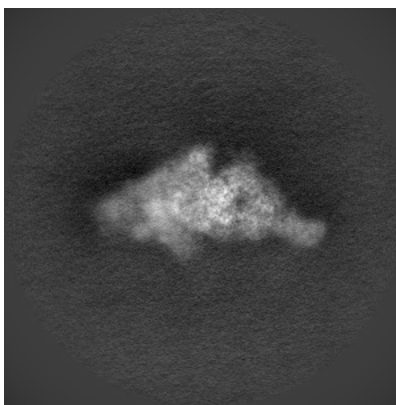


Z

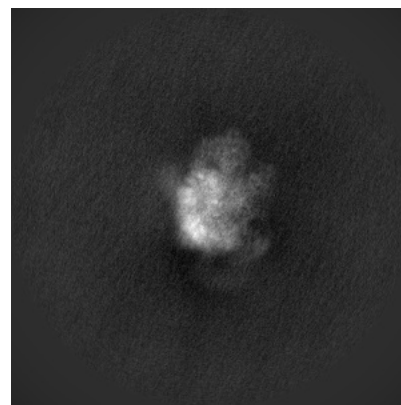
6.1.2 Raw map



X



Y

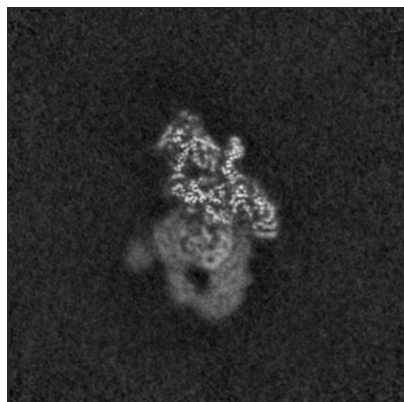


Z

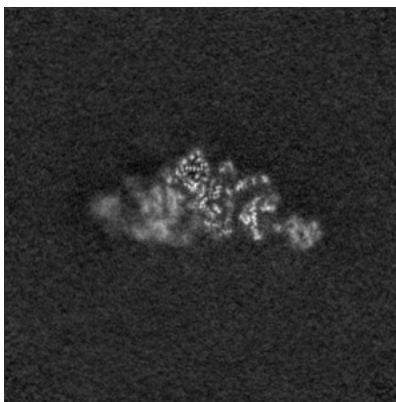
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

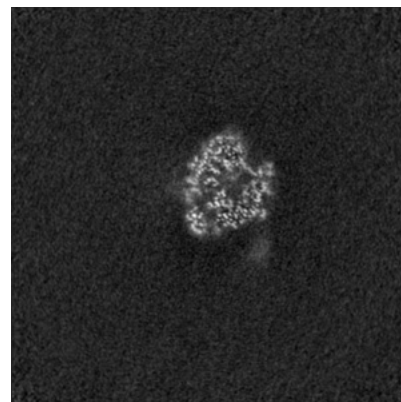
6.2.1 Primary map



X Index: 300

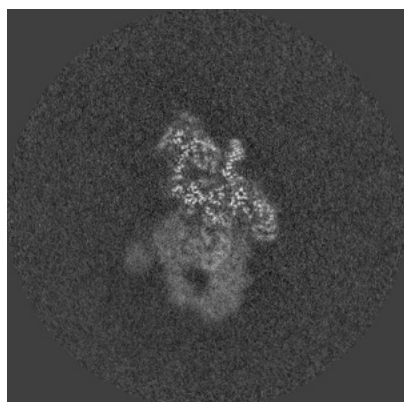


Y Index: 300

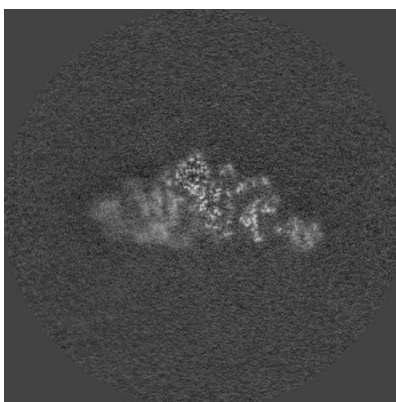


Z Index: 300

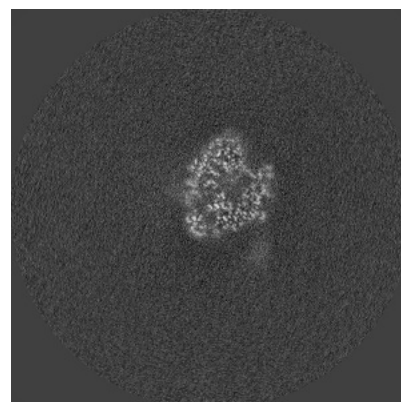
6.2.2 Raw map



X Index: 300



Y Index: 300

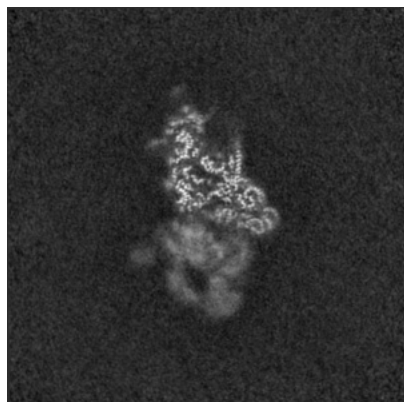


Z Index: 300

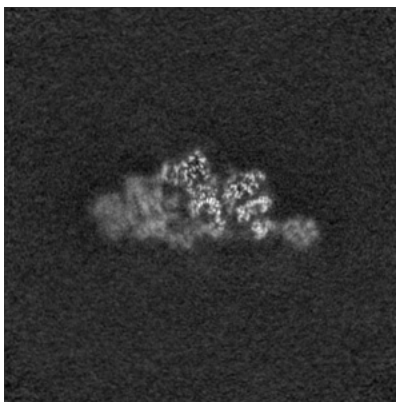
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

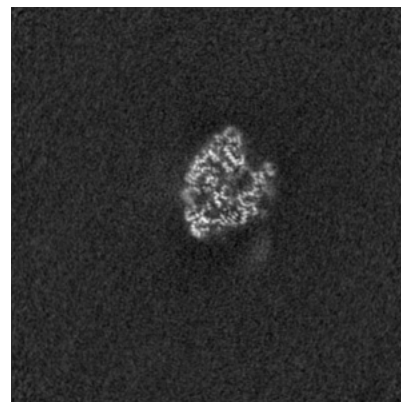
6.3.1 Primary map



X Index: 286

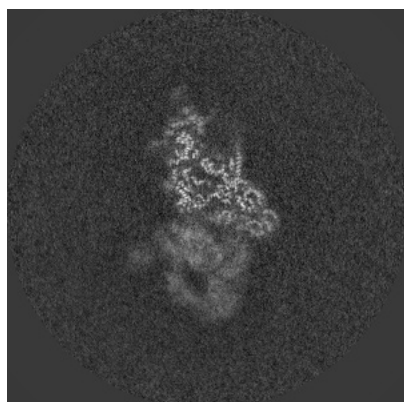


Y Index: 308

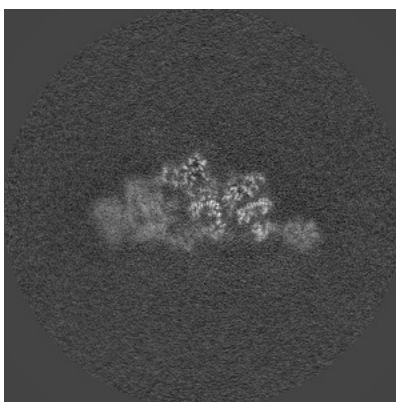


Z Index: 304

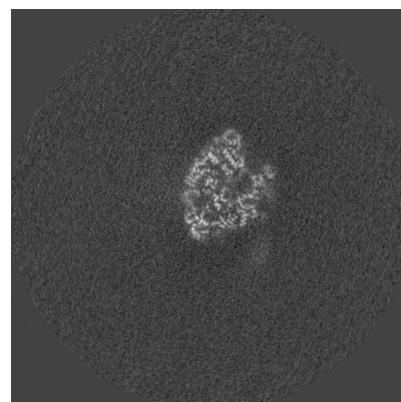
6.3.2 Raw map



X Index: 286



Y Index: 308

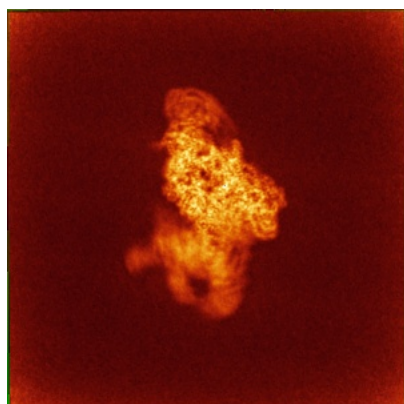


Z Index: 304

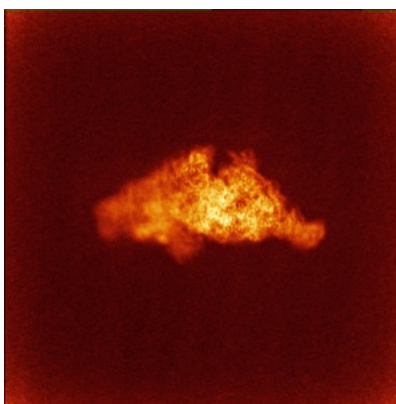
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

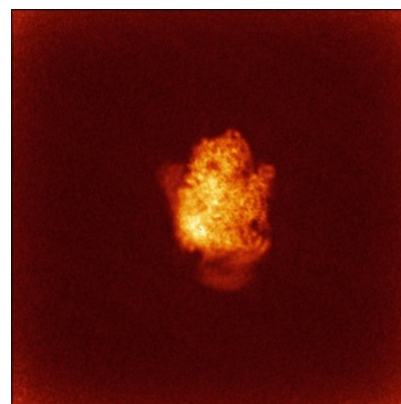
6.4.1 Primary map



X

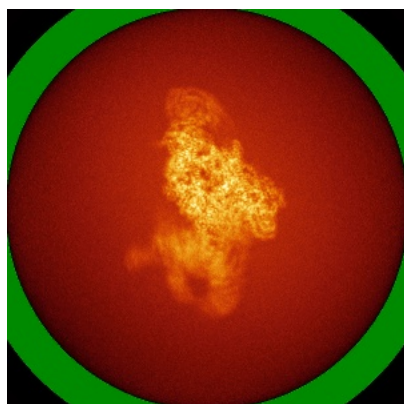


Y

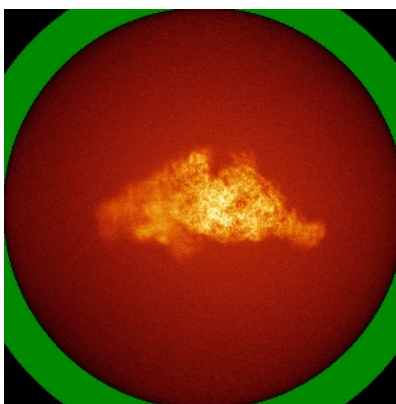


Z

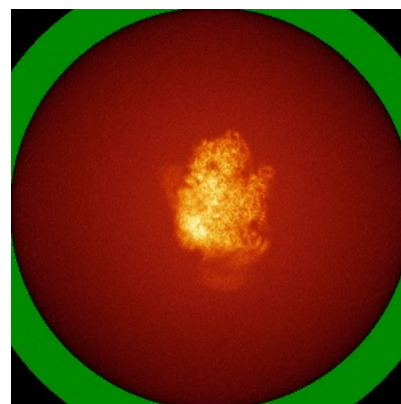
6.4.2 Raw map



X



Y

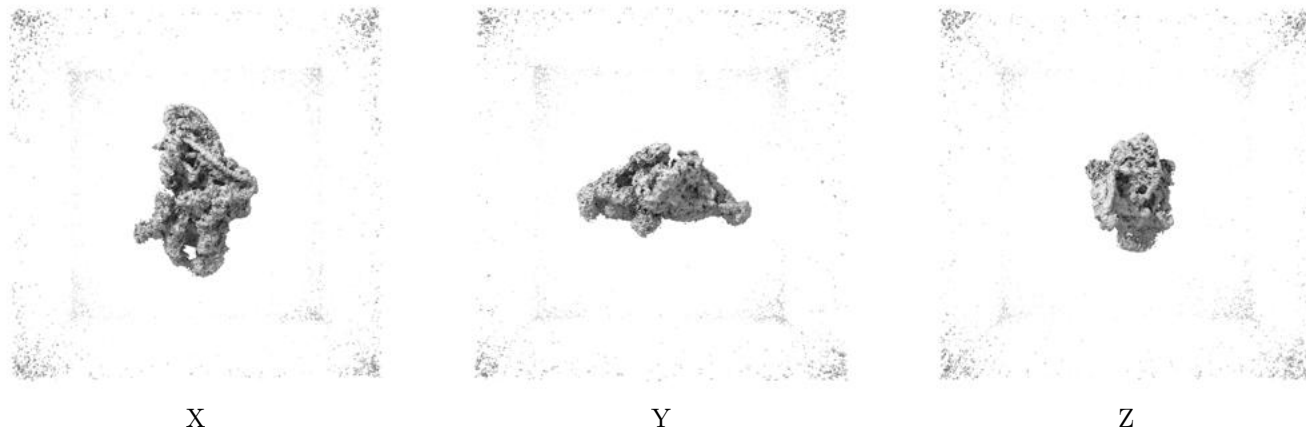


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

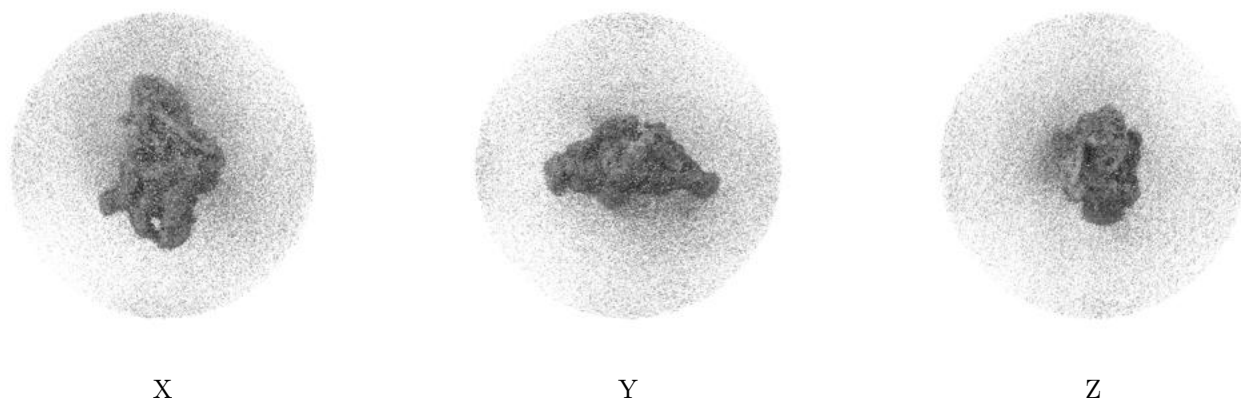
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

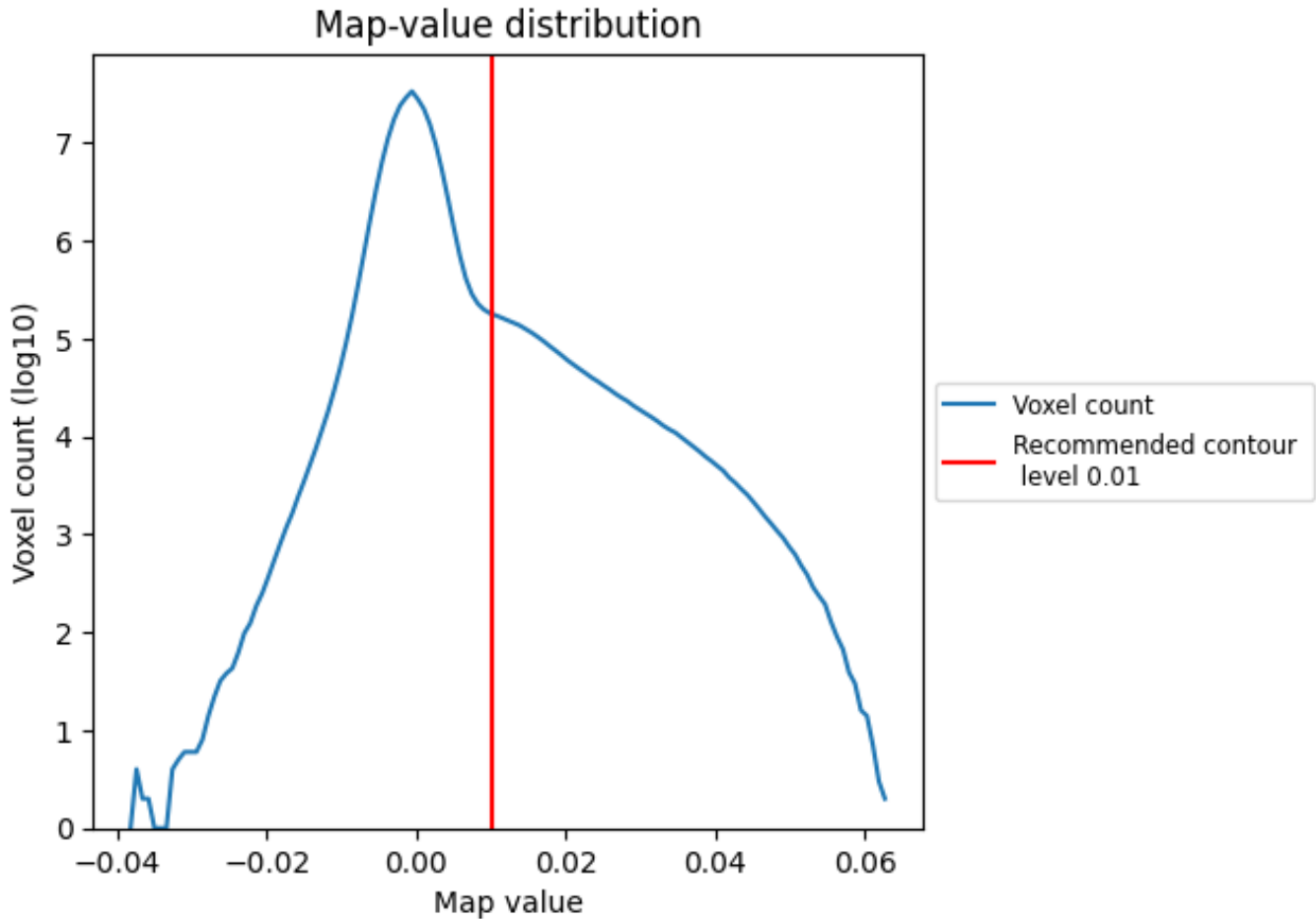
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

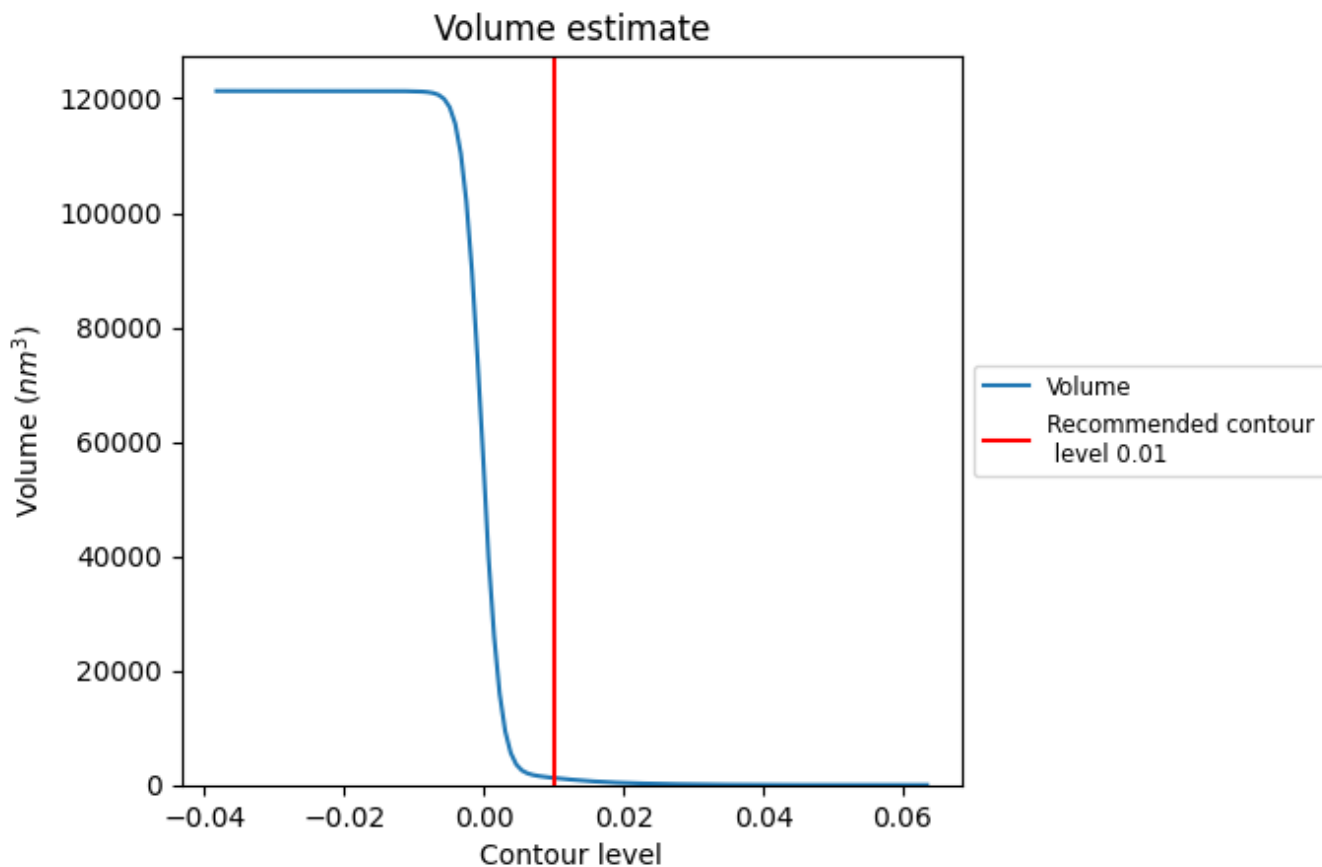
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

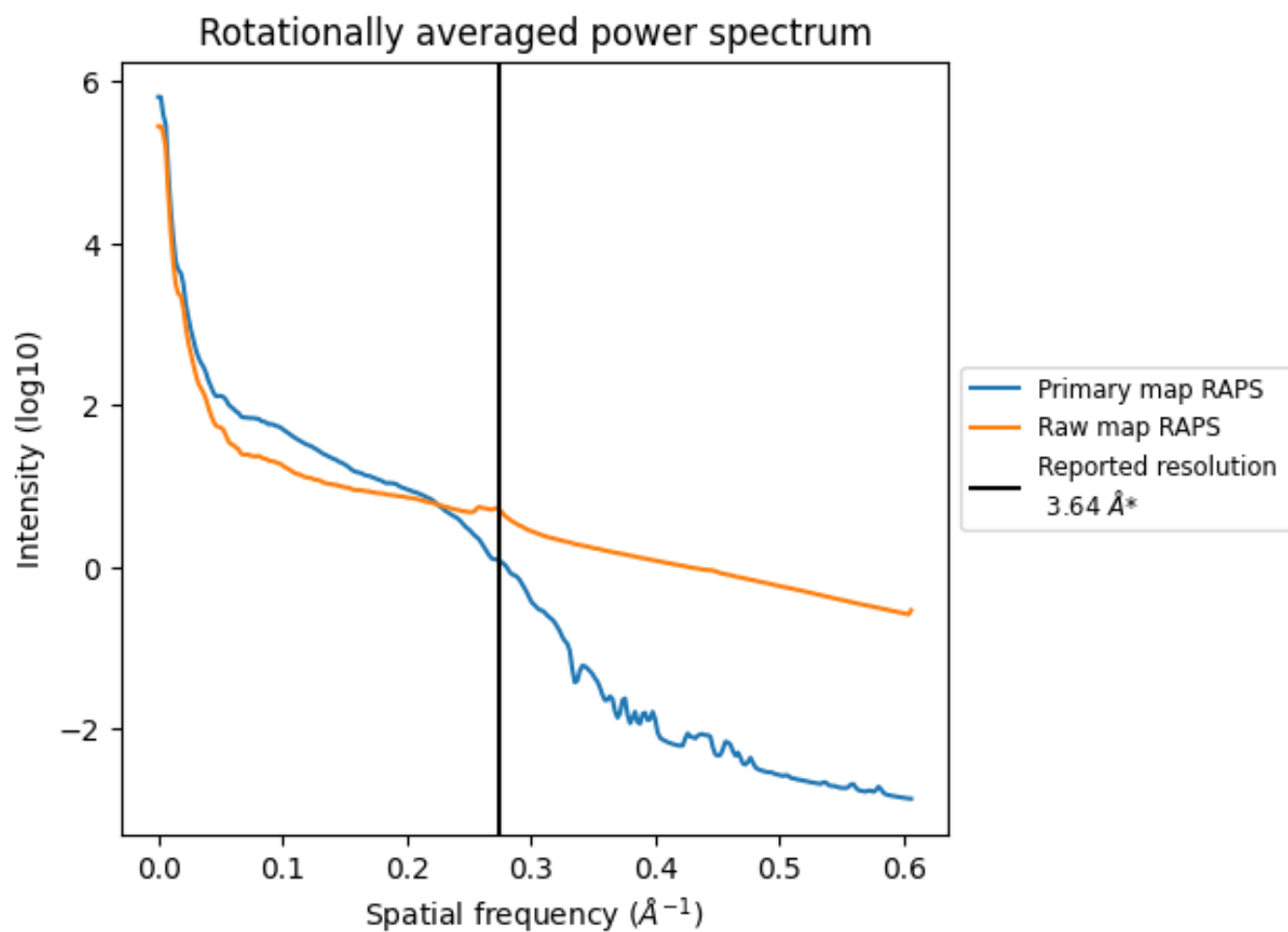
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1237 nm³; this corresponds to an approximate mass of 1117 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

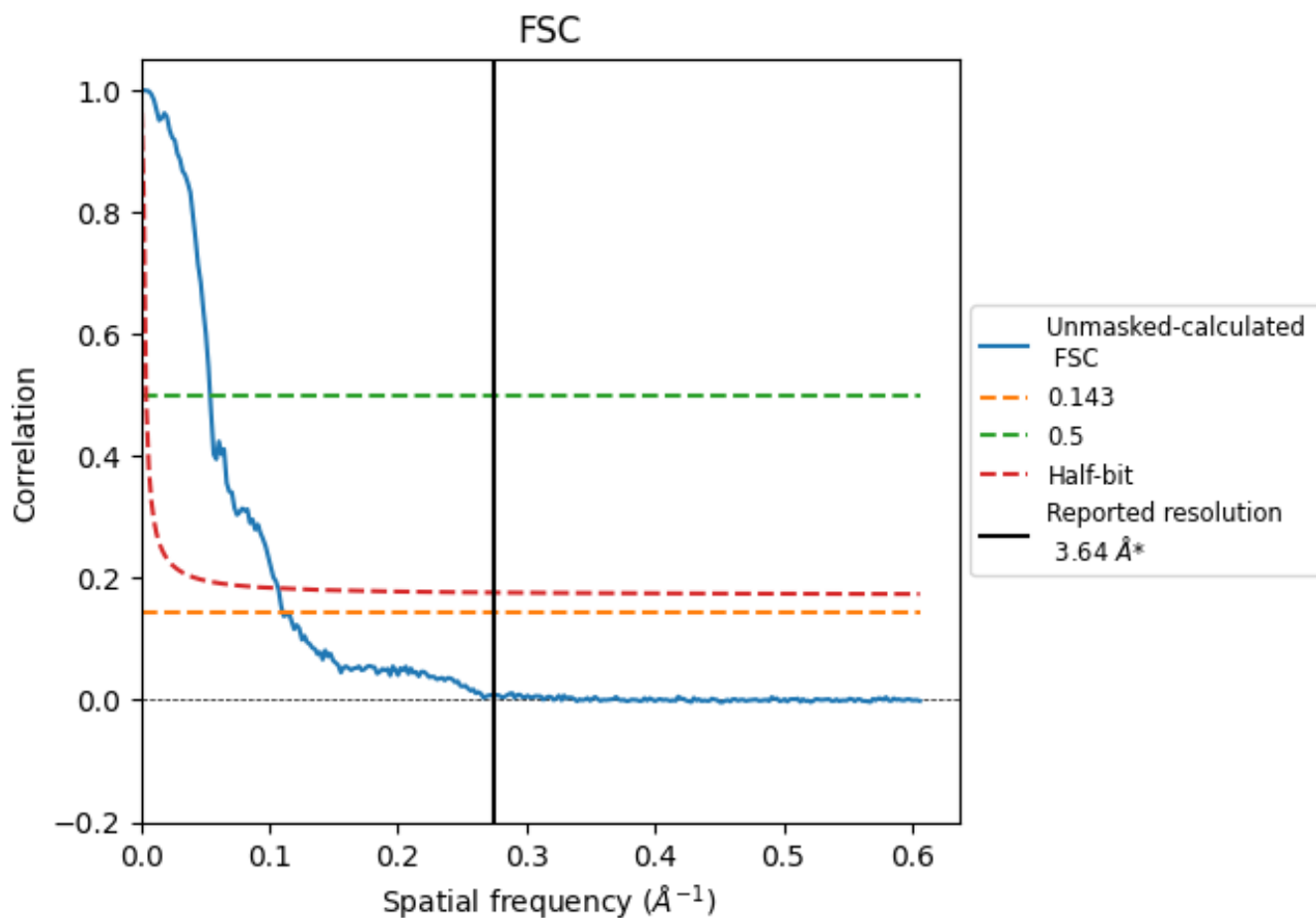


*Reported resolution corresponds to spatial frequency of 0.275 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.275 Å⁻¹

8.2 Resolution estimates [i](#)

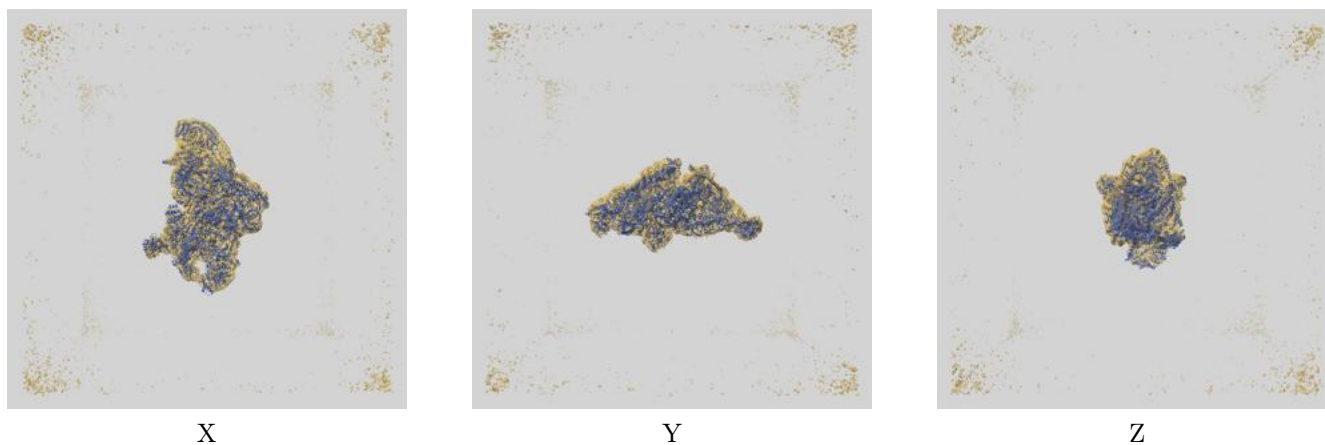
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.06	18.59	9.37

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 9.06 differs from the reported value 3.64 by more than 10 %

9 Map-model fit [i](#)

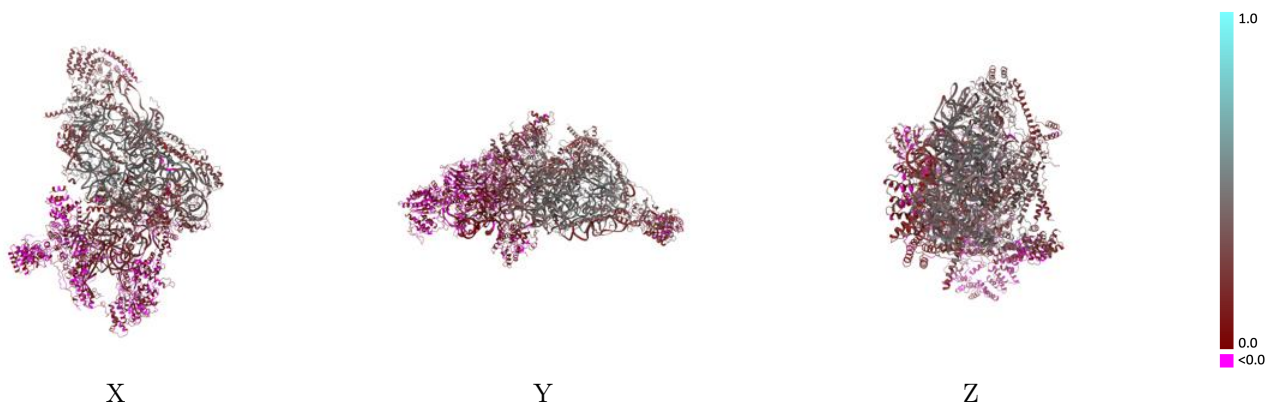
This section contains information regarding the fit between EMDB map EMD-54129 and PDB model 9ROR. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



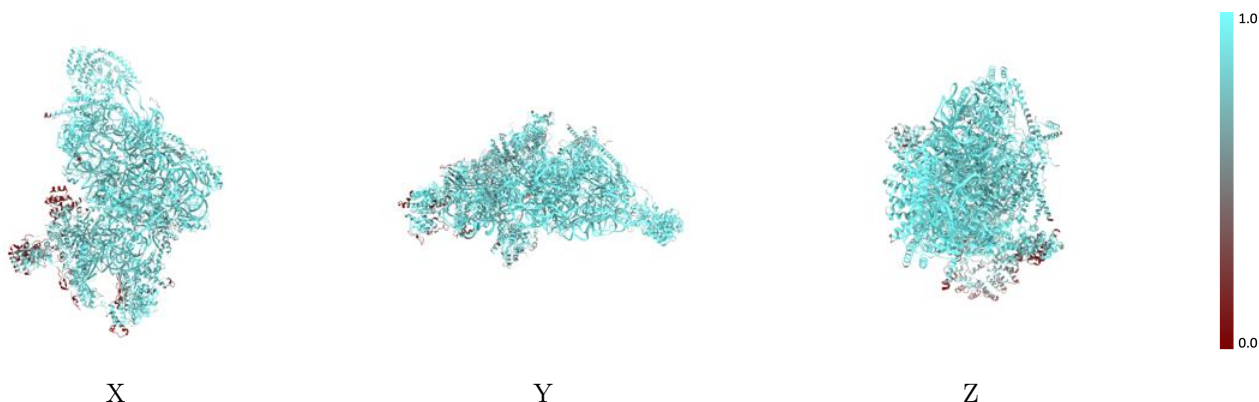
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



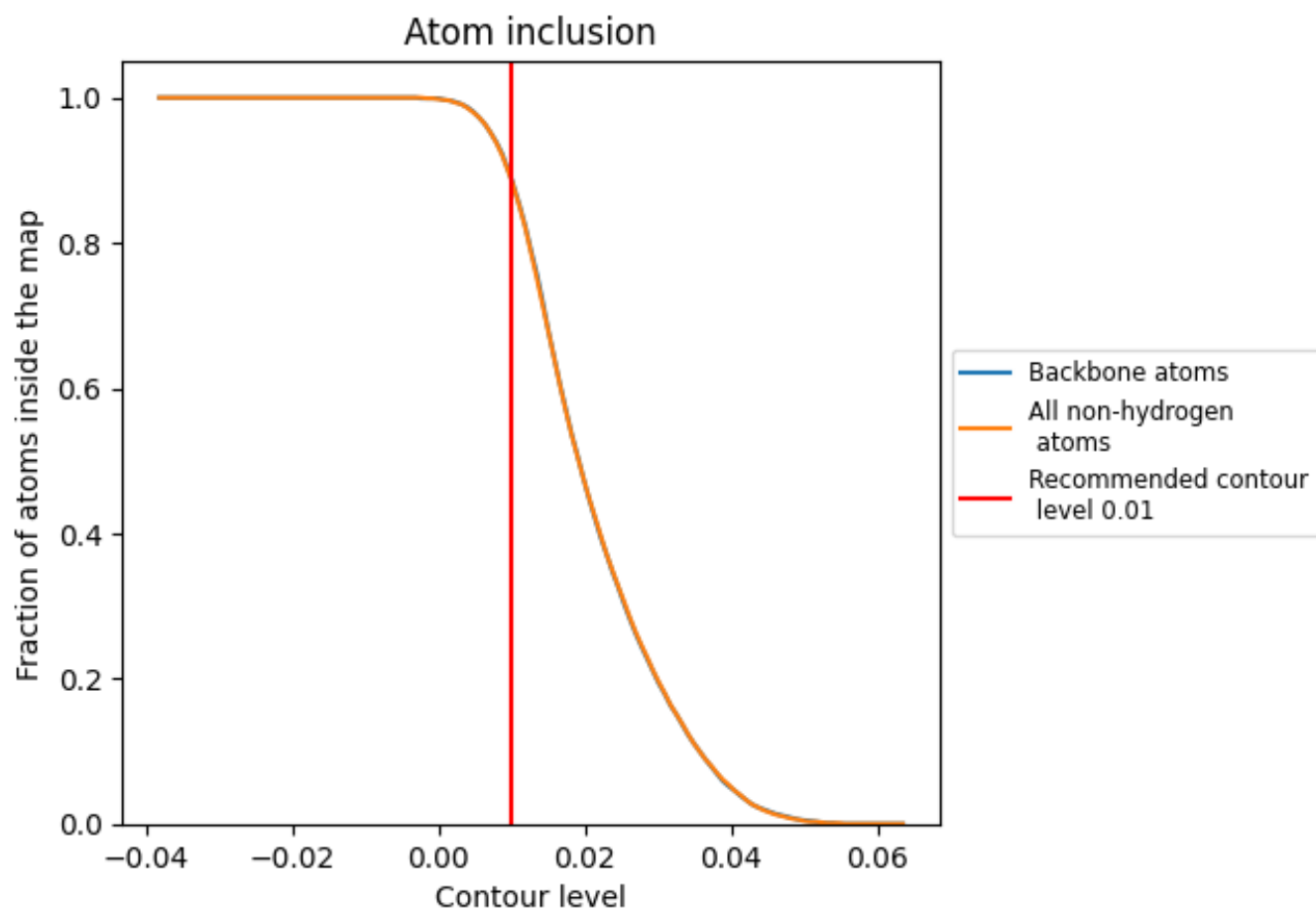
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8850	 0.2510
0	 0.9510	 0.3050
1	 0.7820	 0.0850
3	 0.9210	 0.3780
4	 0.5810	 0.0560
A	 0.9870	 0.3340
B	 0.9050	 0.3110
C	 0.9120	 0.1320
D	 0.8650	 0.3170
E	 0.9230	 0.3390
F	 0.8920	 0.0760
G	 0.8550	 0.1540
H	 0.7870	 0.0610
I	 0.9500	 0.3340
J	 0.9500	 0.4020
K	 0.7890	 0.0700
L	 0.9250	 0.3690
M	 0.9250	 0.4140
N	 0.9610	 0.4420
O	 0.9450	 0.3980
P	 0.9440	 0.3550
Q	 0.9110	 0.3010
R	 0.9080	 0.3570
S	 0.8960	 0.2860
T	 0.9430	 0.4010
U	 0.9010	 0.3140
V	 0.9270	 0.1950
W	 0.9270	 0.2680
X	 0.7980	 0.0410
Y	 0.5180	 0.0310
Z	 0.8710	 0.1120
a	 0.7570	 0.1260
b	 0.8260	 0.1470

